

PB86-144862

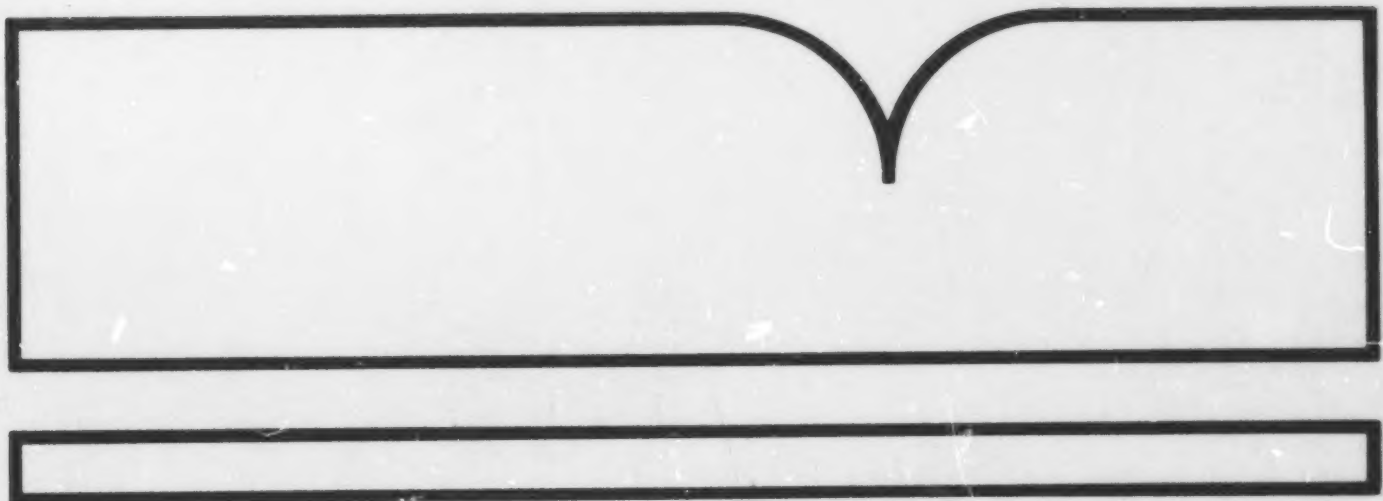
Methods for Mesoscale Modeling for
Materials Damage Assessment
User's Guide

Brookhaven National Lab., Upton, NY

Prepared for

Environmental Protection Agency, Research
Triangle Park, NC

Dec 85



U.S. Department of Commerce
National Technical Information Service

NTIS

PB86-144862

EPA/600/8-85/028
December 1985

METHODS FOR MESOSCALE MODELING FOR
MATERIALS DAMAGE ASSESSMENT
User's Guide

by

F. W. Lipfert, L. R. Dupius, and J. W. Schaedler
Environmental Systems Analysis Group
Brookhaven National Laboratory
Upton, New York 11973

EPA Interagency Agreement DW 931224

Project Officer

Jack L. Durham
Atmospheric Chemistry and Physics Division
Atmospheric Sciences Research Laboratory
Research Triangle Park, North Carolina 27711

ATMOSPHERIC SCIENCES RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
RESEARCH TRIANGLE PARK, NORTH CAROLINA 27711

REPRODUCED BY
NATIONAL TECHNICAL
INFORMATION SERVICE
U.S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

TECHNICAL REPORT DATA (Please read instructions on the reverse before completing)		
1. REPORT NO. EPA/600/8-85/028	2.	3. RECIPIENT'S ACCESSION NO. PB86 T44862 JS
4. TITLE AND SUBTITLE METHODS FOR MESOSCALE MODELING FOR MATERIALS DAMAGE ASSESSMENT User's Guide	5. REPORT DATE December 1985	
	6. PERFORMING ORGANIZATION CODE	
7. AUTHOR(S) F. W. Lipfert, L. R. Dupius, and J. W. Schaedler	8. PERFORMING ORGANIZATION REPORT NO.	
9. PERFORMING ORGANIZATION NAME AND ADDRESS Environmental Systems Analysis Group Brookhaven National Laboratory Upton, New York 11973	10. PROGRAM ELEMENT NO. CCVN1A:05 Task 5066 (FY-86)	
	11. CONTRACT/GRANT NO. IAG DW 931224	
12. SPONSORING AGENCY NAME AND ADDRESS Atmospheric Sciences Research Laboratory - RTP, NC Office of Research and Development U.S. Environmental Protection Agency Research Triangle Park, North Carolina 27711	13. TYPE OF REPORT AND PERIOD COVERED Interim 11/84 - 10/85	
	14. SPONSORING AGENCY CODE EPA/600/09	
15. SUPPLEMENTARY NOTES		
16. ABSTRACT Assessment of acid deposition damage to materials requires as a minimum detailed knowledge of SO₂ (gas) and wet H₂ annual deposition fields on time and space scales consistent with the mechanisms of damage and the distribution of materials at risk. Methods for urban air quality SO₂ modeling are reviewed and a set of simplified algorithms is presented suitable for relatively rapid assessment of a large number of cities. The method is relatively "meteorology free" in that regional wind roses have been incorporated into the parameterization rather than the use of site-specific wind roses. Separate algorithms are presented for point and for area sources, and the model is designed to produce annual average concentration estimates over 5-km grids. The Parameterized Air Quality Model-Annual (PAQMAN), is designed to mimic the performance of the Climatological Dispersion Model (CDM). McElroy-Pooler dispersion coefficients are used for point sources, with Briggs' plume rise, and Pasquill-Gifford dispersion coefficients are used for area sources. PAQMAN results correlated well with CDM calculations for the New Haven-Pittsburgh Metropolitan Statistical Areas (MSAs) with correlation coefficients of 0.90 and 0.80, respectively. Comparisons between PAQMAN and measured concentrations averaged over each MSA were also favorable over the entire spectrum of 112 MSAs.		
17. KEY WORDS AND DOCUMENT ANALYSIS		
a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
18. DISTRIBUTION STATEMENT RELEASE TO PUBLIC	19. SECURITY CLASS (This Report) UNCLASSIFIED	21. NO. OF PAGES
	20. SECURITY CLASS (This page) UNCLASSIFIED	22. PRICE

DISCLAIMER

The information in this document has been funded wholly or in part by the United States Environmental Protection Agency under Interagency Agreement DW 931224 with United States Department of Energy, Brookhaven National Laboratory. It has been subject to the Agency's peer and administrative review, and it has been approved for publication as an EPA document.

Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

Abstract

Assessment of acid deposition damage to materials requires as a minimum detailed knowledge of SO_2 (gas) and wet H^+ annual deposition fields on time and space scales consistent with the mechanisms of damage and the distribution of materials at risk. Methods for urban air quality SO_2 modeling are reviewed and a set of simplified algorithms is presented suitable for relatively rapid assessment of a large number of cities. The method is relatively "meteorology free" in that regional wind roses have been incorporated into the parameterization rather than the use of site-specific wind roses. Separate algorithms are presented for point and for area sources, and the model is designed to produce annual average concentration estimates over 5-km grids. The Parameterized Air Quality Model-Annual (PAQMAN), is designed to mimic the performance of the Climatological Dispersion Model (CDM). McElroy-Pooler dispersion coefficients are used for point sources, with Briggs' plume rise, and Pasquill-Gifford dispersion coefficients are used for area sources. PAQMAN results correlated well with CDM calculations for the New Haven-Pittsburgh Metropolitan Statistical Areas (MSAs) with correlation coefficients of 0.90 and 0.80, respectively. Comparisons between PAQMAN and measured concentrations averaged over each MSA were also favorable over the entire spectrum of 112 MSAs.

ACKNOWLEDGEMENTS

The authors are grateful for the cooperative assistance of several people. Among these are Dr. Joseph Tikvart, EPA/OAQPS, who was particularly helpful and provided modeling consultation on several occasions, Marty Leach BNL/DAS, who assisted with the inclusion of dry deposition with the CDM model. Dr. Ari Patrinos, BNL/DAS, who provided guidance on hydrogen ion deposition and Dr. Jack Shannon, ANL, who provided estimates of regional background SO₂ data. Bob Malone provided data processing and computer assistance, while Donna Cange and Liz Seubert were responsible for typing the manuscript.

CONTENTS

DISCLAIMER.....	ii
ABSTRACT.....	iii
ACKNOWLEDGEMENTS.....	vi
1.0 INTRODUCTION.....	1
2.0 SCOPE OF THE MODELING EFFORT.....	4
2.1 Pollutants to be Considered.....	4
2.2 Time Scales.....	4
2.3 Spatial Scales.....	6
2.4 Accuracy Requirements.....	6
3.0 CONVENTIONAL MODELING METHODS.....	8
3.1 Candidate Models.....	8
3.2 Model Descriptions.....	9
3.3 Model Selection.....	9
3.4 Modification to the CDM Model.....	11
4.0 APPLICATIONS OF THE CDM MODEL.....	14
5.0 MODEL PARAMETERIZATION.....	15
5.1 Point Sources.....	15
5.2 Area Sources.....	17
5.3 Source Allocation Algorithms.....	24
5.4 Emissions Inventory Quality Assurance.....	25
6.0 APPLICATIONS OF THE PARAMETRIC MODEL AND COMPARISON TO CDM RUNS...	26
6.1 New Haven Case Study.....	26
6.2 Pittsburgh Case Study.....	31
7.0 LIMITATIONS OF THE MODEL.....	37
8.0 REGIONAL BACKGROUND AIR QUALITY AND WET DEPOSITION.....	39
8.1 Background SO ₂	39
8.2 Hydrogen Ion (H ⁺) Deposition Estimates.....	39
9.0 CONCLUSIONS.....	42
REFERENCES.....	43
APPENDIX A: WIND ROSE COMPARISONS.....	45
APPENDIX B: PAQMAN USER'S GUIDE.....	50
APPENDIX C: PAQMAN PROGRAM CODE LISTING.....	53

FIGURES

<u>Number</u>		<u>Page</u>
1	Point and Area Source Emission Locations for Parameterized Deposition Calculations.....	12
2	Concentration Ratio vs. Distance Ratio.....	16
3	Maximum Concentration vs. Stack Height.....	18
4	Downwind Distance to Maximum Concentration.....	19
5	Concentration Ratio vs. Distance Ratio.....	20
6	Scale Effect on Area-Source Diffusion.....	22
7	Area Source Algorithm.....	23
8	Schematic of the New Haven Area.....	27
9	Land Use Categories.....	28
10	CDM Computed SO ₂ Concentrations in New Haven, CT.....	29
11	Total SO ₂ New Haven, CT - PAQMAN.....	30
12	Comparison of PAQMAN and CDM SO ₂ Concentration Estimates for New Haven.....	32
13	Comparison of PAQMAN and CDM SO ₂ Concentration Estimates for Pittsburgh.....	34
14	Calculated vs. Measured SO ₂ for Pittsburgh.....	35
15	Background SO ₂ Data.....	40
16	Hydrogen Ion Deposition Isopleths.....	41
A-1	Surface Wind Roses by Stability and Wind Speed.....	46
A-2	Surface Wind Roses by Stability and Wind Speed.....	47
A-3	Surface Wind Roses by Stability and Wind Speed.....	48

TABLES

<u>Number</u>		<u>Page</u>
1	SO ₂ Concentrations in New Haven, CT.....	2
2	Summary of Major Algorithms and Capabilities of Candidate Models.....	10
3	Results of Parametric Deposition Calculations.....	13
4	Regression Analysis PAQMAN vs. CDM Concentrations.....	33
A-1	Wind Rose Statistics.....	49

SECTION 1

1.0 INTRODUCTION

One of the components of the National Acid Precipitation Assessment Program (NAPAP) deals with damage to materials in the built environment. Such an assessment requires detailed information on deposition of corrosive agents, both wet and dry, on scales compatible with urban areas (generally less than 50 km). The atmospheric agents of interest include both acidic gases and contaminated precipitation, as well as particulates in some instances. These agents have important local and regional sources in the populated and industrial parts of North America, especially in the Northeastern quadrant of the U.S., which is the subject of the first (1985) NAPAP assessment of materials damage. The materials damage portion of this assessment focuses on SO_2 (gas) and wet deposition of H^+ , as potentially damaging agents.

The urban scale is probably unique to the materials damage portion of NAPAP, and offers both challenges and opportunities as an interface. The challenge is to provide sufficiently accurate deposition estimates for materials damage for a large number of urban areas (ca. 250) within very limited time and cost constraints. The opportunity presented to the remainder of the assessment program is that such detailed consideration of urban sources and deposition will automatically provide sub-grid scale detail to the regional source-receptor considerations that will aid both in pollutant budget balancing and in quality assurance (QA) of the emissions inventory at the local level.

Although the 1985 NAPAP Assessment requires only a description of the current status of damages (and thus deposition), we have elected to employ a methodology that also allows detailed consideration of source-receptor relationships for use in future control strategy design efforts. Thus the urban scale model to be developed can naturally be adopted as a sub-grid scale feature of mesoscale and regional scale models being developed elsewhere to deal with both wet and dry deposition simultaneously. At this time, on the urban scale, the two deposition processes will be considered in an uncoupled fashion. The time scale of interest is the annual average, as discussed in more detail below.

The specific objectives of this work are to:

1. Develop an estimation method for annual average atmospheric SO_2 concentration distributions in urban areas based on monitoring and simple gaussian modeling.
2. Apply this methodology to several Metropolitan Statistical Areas (MSA) in which materials distributions are derived for the 1985 Assessment.
3. Develop data for regional SO_2 background (non-urban) consistent with the urban SO_2 data.
4. Develop and apply a method for estimating urban H^+ (wet) deposition.

5. Develop suitable interfaces between this methodology and the mesoscale and Eulerian models being developed elsewhere.

The corrosion damage functions to be used in the assessment require spatial distributions of two pollutants: gaseous SO_2 and wet deposition of hydrogen ion (H^+), (see below). In neither case are extant monitoring data adequate to characterize the details within metropolitan areas. The sum of the damages in an urban area will be the spatial integral of the joint distribution of materials at risk and deposition, neither of which is uniform in space.

Sulfur dioxide monitors tend to be located to meet regulatory needs, i.e., to determine compliance with National Ambient Air Quality Standards (NAAQS). As a result, monitors tend to be sited around large point sources of emissions and in the densest portions of urban areas. In many cases, an urban area will contain only a few monitors, an inadequate basis to characterize the distribution of air quality within the city. Table 1 presents data for New Haven, CT, to illustrate this point. It can be seen that use of the measured value would greatly overstate the SO_2 concentrations appropriate for estimating materials damage.

TABLE 1. SO_2 CONCENTRATIONS IN NEW HAVEN, CT ($\mu\text{g}/\text{m}^3$)
(Based on background of $16.8 \mu\text{g}/\text{m}^3$)

1. Measured value (1978)	37.2
2. Maximum calculated value	31.6
3. Area-average concentration	19.7
4. Population weighted concentration	22.1
5. Painted surface area weighted concentration	21.1
6. Galvanized steel surface area weighted concentrations.	23.5

Because of the emphasis on annual average estimates and because of the need for simple, expedient methods, the gaussian plume model is the prime candidate. There have been many reviews and evaluations of gaussian plume modeling methods. The Environmental Protection Agency has selected a number of them for official regulatory use and designated them as "Guideline Models" (1). Various features of such models are discussed below. The shortcomings of these models have also been the subject of extensive review and evaluation (2). It seems safe to say that the main stream of air pollution dispersion model development is towards more complicated models; the present effort aimed at simplification is thus something of an anachronism.

The gaussian plume equation is an analytic solution of the advection-diffusion equation and can be solved in closed-form if analytic

power-law expressions are used for the dispersion factors σ_x and σ_y . Lipfert developed some closed-form solutions (3) for maximum short-term (1-24 hr) average concentrations for point sources on this basis; such parametric-type studies have been done by others as well (4). However, in general, less interest has been given to annual average estimation methods, in part because of the need to use wind roses as inputs, making analytic solutions difficult, if not impossible.

For area sources, simplified methods range from simple box models (5) to repetitive numerical integration of a gaussian line source model (6). In recent years following implementation of the Clean Air Act of 1970, interest in area source modeling problems seems to have waned as most U.S. cities came into compliance with primary ambient air quality standards.

The basic approach to simplified modeling presented below is one of parameterization. Simple closed-form algorithms are developed which mimic the performance of a Guideline model, and thus provide a link with current regulation and, it is hoped, physical reality. Monitoring data are used as a guide in this latter regard.

The sections of this report presented below deal with the scope of the effort, a discussion of available candidate gaussian models, the role of dry deposition calculations, the parameterization methods used and their performance on a test case, and finally a discussion of limitations of the approach and recommendations for further research.

SECTION 2

2.0 SCOPE OF THE MODELING EFFORT

The objective is to develop methods for estimating both dry and wet deposition for application to a large number of urban areas. As with most modeling methods, balance must be sought among simplicity of application, accuracy, and resolution of detail. After completion of this first assessment, sensitivity analysis may be used to further refine this balance.

2.1 POLLUTANTS TO BE CONSIDERED

For the initial NAPAP assessment, the pollutants of interest are defined by the available damage functions, which relate the rate of materials deterioration to the concentrations of harmful agents in the atmosphere. These agents are currently limited to SO_2 (gas) and wet deposition of hydrogen ion (H^+). Other substances in the atmosphere are known to be harmful to certain materials, such as particulate matter including acidic aerosols, ozone, NO_x , H_2S , etc. As materials damage testing programs progress and mature, damage functions may become available for some of these other agents, and appropriate deposition estimation methods would then be required. These requirements would then be interfaced with the Regional Acid Deposition Model (RADM), being developed elsewhere, which deals with the full chemistry of the atmosphere.

2.2 TIME SCALES

Like many other effects of acid deposition, corrosion is a long term process that integrates the cumulative effects of many repetitive attacks on exposed surfaces. At issue then is whether an estimate of long term (annual average) deposition is sufficient to describe the cumulative effects. Tests have shown (7) that some metals exhibit a "memory" effect--the conditions of first exposure of a fresh surface affecting the initial corrosion rate have an effect on subsequent corrosion.

However, the NAPAP assessment deals with current levels of damage to the existing built environment, which by and large is not composed of fresh surfaces. Long term steady state corrosion rates are thus of primary interest, although there may also be interest in projecting remaining lifetimes of specific important monuments and other cultural resources. For this purpose, we plan to estimate "current" damage based on steady state annual corrosion rates, in turn based on "current" emissions as found in the NAPAP inventory (discussed further below).

A further temporal consideration deals with the intermittent nature of SO_2 deposition, which has been shown (8) to be greatly enhanced when surfaces are wet, either from condensation or precipitation. In most locations in the Northeast, the former will dominate; precipitation times account for a small fraction of the total, say 3-5% (9). The question arises as to whether the annual average SO_2 concentration is a good estimate of the average concentration during times of heavy deposition.

In order to address this question, data on hourly SO_2 concentrations measured by four different types of continuous analyzers¹ were obtained from ten sites in New York State during 1977 from the New York State Department of Environmental Conservation. Hourly values of relative humidity (RH), temperature, wind speed and precipitation were also recorded. The hypothesis to be evaluated here is that hours of high relative humidity (sufficiently high to promote condensation on metal surfaces) would be associated with lower than average SO_2 . Logs of the SO_2 were used in the analysis since it was anticipated that the distribution of their concentrations would be more nearly normal.²

There were 17 combinations of sites and SO_2 instrument types with sufficient data to be evaluated. Eight of these showed average SO_2 concentrations that were clearly lower during hours of $\text{RH} > 90\%$. Several stations showed indications of possible miscalibration of humidity instruments as manifested by either too few or too many hours of $\text{RH} > 90\%$ (or $\text{RH} = 100\%$), making strict comparisons among sites somewhat difficult. Too few hours of high indicated RH would make it difficult to obtain a reliable subset average (2 sites). Too many hours of high indicated RH would blur the distinction and tend to make the subsets identical (2 instances). However, in this latter situation, a significant negative correlation between SO_2 and RH could be taken as acceptance of the hypothesis (4 cases).

Failure to find the expected inverse relationship between RH and SO_2 concentrations in some instances may be related to the concurrent relationships between SO_2 and temperature (usually negative) and between temperature and RH (usually negative). In fact, the largest SO_2 difference was found in Manhattan where the RH-temperature relationship was positive, probably due to urban perturbations. In some cases, there were inconsistencies in SO_2 behavior at the same site, as indicated on different instruments, suggesting that data reliability may also be a problem.

Other subsets that were identified were the hours with more than 0.01 inches of precipitation recorded and the hours with ambient temperature 65°F or less, during which space heating might be expected. The precipitation hours all had average SO_2 lower than their respective total data sets, as expected, thus indicating a certain degree of reliability to the data. The space heating hours did not all have high average SO_2 , indicating that in some instances there were important sources of SO_2 other than space heating. Presence or absence of space heating SO_2 sources did not appear to be a reliable predictor for SO_2 gradients due to humidity.

The final analysis of these data consisted of multiple regressions of (log) SO_2 with wind speed, RH, ambient temperature, and precipitation. 14 out

¹Automated West-Gaeke colorimetric (10 sites), coulometric (5 sites), pulsed fluorescence (1 site), second-derivative spectroscopic (1 site).

²This analysis appears in Wyzga and Lipfert, 1985 (10), and was partially supported by the Electric Power Research Institute.

of 17 regressions showed negative regression coefficients ($\log SO_2$ on RH) as expected; nine of these were statistically significant ($P < 0.05$). Of the three regressions with positive RH coefficients, two were with small data sets and one was an apparent RH miscalibration situation with a large number of 100% RH data points.

Thus, we have found evidence of an independent RH effect on SO_2 concentration, which could be due to absorption of SO_2 in condensation on surfaces or due to accelerated conversion of SO_2 to SO_4 aerosol. Based on an approximate difference of twenty points in relative humidity between the annual average and the critical humidity at which corrosion is accelerated, the average regression coefficient indicates that the SO_2 concentration during times of corrosion would be about 9% lower than the annual average SO_2 , all other factors being equal. However, in most cases, these other factors are not equal, and thus the overall average SO_2 concentration may still be a good estimator to be used in corrosion studies. For this reason, it appears to be acceptable to base the assessment on annual average SO_2 concentrations.

2.3 SPATIAL SCALES

The scales of interest for materials damage range from that of an individual monument (1 m) or other cultural resource to that of an entire metropolitan area (~ 50 km). The latter is the more general case, and it should be pointed out that damage to common construction materials is of interest to the assessment only in the aggregate, as an economic input to the cost-benefit equation. The required integrals are those of the joint spatial distributions of the materials at risk and the concentration fields. Neither distribution tends to be uniform over an urban area; furthermore, the distribution of relative humidity, which controls surface wetness and thus SO_2 deposition rates, will also be non-uniform in major metropolitan areas. Thus, the spatial scale for air quality modeling must be considered in conjunction with the resolution of the inventory of materials at risk.

The basic geographic units for this inventory are census tracts, which vary in size from say 0.25 km^2 to 50 km^2 or more. However, since stratified random sampling is used in developing the inventory, the contents of specific tracts are inventoried or characterized in a generic sense only. In the larger residential tracts, spatial homogeneity may not be a bad assumption. However, we will not have the ability to predict the exact location or characteristics of specific central business district features. Thus aggregation of densely built center city tracts is not only permissible but advisable.

A final consideration is computing resources. A gridded calculation system is planned, as discussed below, and the size of each grid cell has a squared effect on computational time. A $5 \times 5 \text{ km}$ grid cell was selected as providing a reasonable compromise between precision and computing resources, as discussed below.

2.4 ACCURACY REQUIREMENTS

The accuracy requirements of this modeling scheme must be keyed to the present state-of-the-art, its application, and the accuracy of the other

elements of the assessment that will contribute to the final damage estimates. The accuracy of gaussian models is commonly stated as within a factor of two, 50% of the time (2), although annual averages should be considerably better, especially if keyed to the available monitoring data. Parameterization of a model thus should not be allowed to appreciably degrade this performance. On this basis, an accuracy goal (with respect to the "parent" model) of $\pm 25\%$ seems reasonable.

A further consideration is the role of background air quality in contributing to the overall corrosion or damage rates. In the Northeast, background SO_2 is often an appreciable part of the total concentration, except near urban hot spots. MSA-averaged SO_2 monitoring data were compared to ASTRAP-computed¹ regional background, for the 109 Northeastern MSA's with monitoring data. 16 of these had measured values less than background, an average ratio of 0.91. Since these locations were mostly smaller MSA's, this serves as a check on the validity of the ASTRAP calculations. For the locations where measured SO_2 exceeded background, an average ratio of 1.80 was found. In other words, for these locations, 55% of the SO_2 was from regional background sources. For the whole data set of 109 MSA's, 60% of the SO_2 was from regional background.

If background is 50% of the total concentration, then modeling accuracy requirements may be eased somewhat, realizing that the background estimates will have their own, probably unknown, variance.

There are considerable uncertainties in the other elements of the damage assessment equation. Damage functions are capable of predicting material lifetimes only within about a factor of two, although the precision of individual pollutant coefficients tends to be much better (11). Materials inventories are also uncertain, to a degree yet to be determined. Thus the final modeling accuracy requirements must be reviewed after all the assessment elements have been assembled and evaluated.

¹Computations made by Dr. Jack Shannon of Argonne National Laboratory, using the Advanced Statistical Trajectory Model (ASTRAP).

SECTION 3

3.0 CONVENTIONAL MODELING METHODS

There are several approaches to mathematical modeling of atmospheric dispersion, each with its own set of physical assumptions. These range from steady-state gaussian type models to more complicated methods, such as grid trajectory and particle-in-cell models, which solve the advection-diffusion equation numerically. Each approach has its advantages and disadvantages, depending upon the situation to which they are applied. Gaussian models are relatively easy to use, with minimum data input and reasonably moderate computer storage and usage requirements. However, they are based upon simplistic assumptions of spatial and temporal uniformity of meteorological conditions, and constant pollutant emission rates. Numerical models, on the other hand, can provide more realistic estimates over short time periods, but require large amounts of input data and computer storage.

In spite of the underlying simplicity inherent in their application, gaussian models are the most widely used for modeling atmospheric dispersion. In fact, most of the current models recommended by the U.S. EPA (1) are gaussian. Therefore, since long-term impacts (annual average pollutant concentrations) are of primary interest here and since estimates for several urban areas will be needed, the gaussian model is a logical approach.

3.1 CANDIDATE MODELS

Four gaussian-type models were considered for this assessment: Brookhaven National Laboratory Long-Term Gaussian Dispersion Model (12) (BNL), the Air Quality Display Model (13) (AQDM), the Climatological Dispersion Model (14) (CDM) and the Industrial Source Complex Model (15) (ISC). The latter two are EPA-approved Guideline models. All of these models are based upon the same physical assumptions and basically use similar mathematical formulations to calculate the annual ground-level concentrations from point and area sources. Emissions data are used in conjunction with a joint frequency distribution of wind speed, wind direction and atmospheric stability in the climatological form (sector-averaged) of the gaussian plume equation. For point sources, the average concentration (χ_p) at a given receptor is:

$$\chi_p = \frac{16}{2\pi} \sum_n \sum_l \sum_m \phi(k_n, l, m) Q_n S(\rho_n, z; U_l, P_m), \quad (1)$$

where: n = number of point sources
 k_n = wind direction sector
 Q_n = emission rate of the n^{th} point source
 ρ_n = distance from the receptor to the n^{th} point source
 $\phi(k_n, l, n)$ = joint frequency distribution function of wind direction, wind speed and stability class
 m = stability index
 l = wind speed class index

$S(\rho, z; U_\ell, P_m)$ = vertical dispersion function
 z = height of receptor above ground level
 U = wind speed at stack elevation
 P_m = stability category.

For area sources, the average concentration at a given receptor is given by:

$$\chi_A = \frac{16}{2\pi} \int_0^\rho \sum_k q_k(\rho) \sum_{\ell, m} \Phi(k, \ell, m) S(\rho, z; U_\ell, P_m) d\rho \quad (2)$$

where: $q_k(\rho) = Q_A(\rho, \theta)$ over the k^{th} sector, which = area source emission strength.
 Q_A = emission rate per unit area (emission density) of the area source element at radial distance, ρ and wind direction, k , from the receptor.

3.2 MODEL DESCRIPTIONS

The principle algorithms used within each model are summarized in Table 2. The Pasquill-Gifford (P-G) dispersion curves are used in CDM, AQDM, and ISC to describe vertical dispersion; the BNL dispersion curves, based on a system of stability classification according to gustiness, are applied in the Brookhaven Model. Plume rise is calculated according to Briggs (16, 17) (for point sources only), except in the AQDM which uses the Holland plume rise equation (18). None of the models allow for the effects of complex terrain (terrain elevation greater than the plume height). Corrections to account for terrain were not considered in this assessment study.

The major differences among the models are in the treatment (numerical integration) of area sources. Only sources which lie directly upwind of a receptor are assumed to make a contribution to the ground-level concentration of any given receptor in the CDM model (narrow plume hypothesis). Numerical integration is performed using the trapezoid rule. The AQDM model converts area sources to equivalent or "virtual" point sources, and modifies source emission rates by the ratio of the portion of a source area which lies within a 22 1/2-degree sector upwind of a given receptor. Area source contributions in the ISC model are based upon equations for a finite crosswind line source, while area sources are evaluated analytically in the BNL model, which offers a closed-form solution to the area source equation and can save on extensive computer iterations.

3.3 MODEL SELECTION

Since all four models operate rather similarly, the choice of which model to use in developing our parameterization algorithm narrowed down to the model that has been most applied to long-term dispersion modeling in urban areas and is readily accepted within the air quality modeling community. For the most part, the ISC model is usually applied to a group or complex of industrial sources and has not been widely used to model large urban areas. The AQDM is actually the predecessor to CDM and the models are quite similar. However, Turner et al. (19) concluded that AQDM tends to overpredict concentrations more

TABLE 2. SUMMARY OF MAJOR ALGORITHMS AND CAPABILITIES OF CANDIDATE MODELS

ALGORITHM	CDM	AQDM	BNL	ISCLT
Time Averaging Short-term	--	1,3,24-h by Larson's stati- stical technique		
Long-term	Annual average	Annual average	Annual average	Annual average
Plume Rise	Briggs (16)	Holland (18)	Briggs (17)	Briggs (17)
Vertical Wind Profile	Power-law extrapolation	--	Power-law extrapolation	Power-law extrapolation
Initial Dilution Horizontal (σ_{y0}) Vertical (σ_{z0})	-- For $h_s < 50m^*$	-- --	-- --	-- Virtual dis- tances for σ_{z0}
Dispersion Coefficients Horizontal (σ_y) Vertical (σ_z)	Sector-averaging P-G curves	Sector-averaging/ smoothing w.r.t. adjacent sectors P-G curves†	Sector-averaging/ smoothing w.r.t. adjacent sectors. BNL curves	Sector-averag- ing P-G curves (rural) McElroy-Pooler curves (urban)
Mixing Height	Stability-depen- dent modification to Holzworth (20) values	Stability-depen- dent modification to Holzworth (20) values	Stability-depen- dent modification to Holzworth (20) values	Seasonal average maxi- mum and mini- mum heights.
Removal Processes	Exponential decay rate (function of pollutant 1/2- life)	--	Exponential decay rate surface deposition	Surface deposition
Terrain	Flat terrain	Flat terrain	Flat terrain	Terrain $< h_s$
Area Sources	Narrow plume hypothesis trape- zoidal rule of numerical inte- gration	Equivalent virtual point sources	Analytical evalu- ation closed form solution	Finite cross- wind line sources

*Algorithm removed when McElroy-Pooler dispersion curves are applied.

†McElroy-Pooler coefficients were used for point sources in urban areas.

--Not accounted for in model.

than CDM and thus recommends the use of CDM in preference to AQDM. For these reasons, the choice was narrowed to the BNL and CDM models. Several test case (point and area source) runs showed that these two models predicted similar concentrations under a variety of different input assumptions. However, because of its acceptance as a standard EPA regulatory model and extensive previous applications to urban areas, the CDM model was selected for the assessment study.

3.4 MODIFICATIONS TO THE CDM MODEL

3.4.1 Urban Mode Modifications

In its conventional mode, CDM uses the P-G dispersion curves to describe vertical plume dispersion. These curves were derived from experiments performed in smooth, rural, flat terrain, and may not be applicable to dispersion characteristics in urban areas. Therefore, different schemes were utilized to account for increased turbulence. One consists of increasing the P-G stability category by one class (toward decreasing stability), which is built into CDM. The other involved the use of the McElroy-Pooler dispersion coefficients (for point sources only) in keeping with most recent EPA policy for urban areas (1). The latter option was utilized for point sources within the SMSA grid.

3.4.2 Dry Deposition

Presently, the CDM model calculates ground-level concentrations according to Equation (1) for point sources and Equation (2) for area sources. The dispersion function, S, in both cases contains an exponential function of half-life designed to include the removal of pollutants by chemical and physical processes, as follows:

$$R = \exp \left(\frac{-.692 \rho}{U_l T_{1/2}} \right), \quad (3)$$

where: $T_{1/2}$ = pollutant half-life
 ρ = distance from source to receptor
 U_l = wind speed at source height.

The half-life algorithm has been shown to match model prediction reasonably well with measurements. We currently use a 3-hour half life for SO_2 , which accounts for dry deposition, conversion of SO_2 to SO_4 aerosol, and wet deposition. For the purpose of accounting for SO_2 budget terms, it is desirable to explicitly estimate the dry deposition portion directly.

To calculate the dry deposition explicitly, a dry deposition velocity, v_d , is defined which allows the calculation of a deposition flux proportional to the local air concentration at reference height, z_d :

$$F_d(x,y) = v_d \chi(x,y,z_d) \quad (4)$$

In order to account for upwind deposition, which reduces the amount of material available for deposition at a given location, a source-depletion model is used. The concentration from point sources at a given receptor then becomes:

$$\bar{C}_p = 16/2\pi \sum_n \sum_l \sum_m (k_n, l, m) \frac{[Q_n - \int_0^{\rho} v_d \bar{C}(\xi, z_d) d\xi] S(\rho, z, U_l, P_m)}{\rho} d\rho \quad (5)$$

and from area sources is:

$$\bar{C}_A = \frac{16}{2\pi} \int_0^{\infty} \sum_k [q_k(\rho) - \int_0^{\rho} v_d \bar{C}(\xi, z_d) d\xi] \sum_l \sum_m \phi(k, l, m) S(\rho, z; U_l, P_m) d\rho. \quad (6)$$

The deposition integrals in equations (5) and (6) are approximated by

$$\int_0^{\rho} v_d \bar{C}(\xi, z_d) d\xi = \sqrt{2\pi} v_d \sigma_y \bar{C} \rho \quad (7)$$

which is the analytical solution to the integral if C is not a function of distance. In numerical terms, this means holding the concentration constant during any single space step.

This technique was tested with various parametric calculations using four point sources and a single area source. Source locations and parameters are shown in Figure 1.

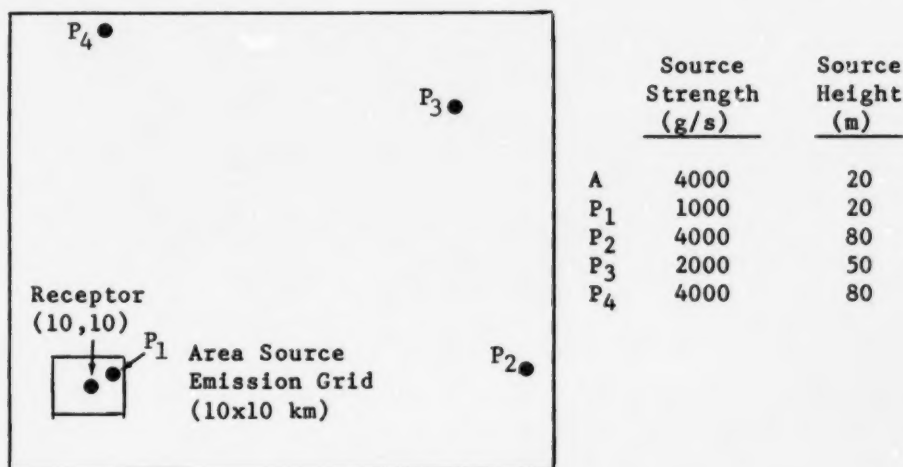


Figure 1. Point and Area Source Emission Locations for Parametric Deposition Calculations

The air concentration and deposition flux were calculated on a square grid every 5 km. For the purposes of this discussion, the results are presented for one receptor only, that located at (10,10) (see Figure 1). Two different wind speeds were used, 1.5 m/s and 12.5 m/s. The results are presented in Table 3.

TABLE 3. RESULTS OF PARAMETRIC DEPOSITION CALCULATIONS

v_d (m/s)	U(m/s)	C_a ($\mu\text{g}/\text{m}^3$)	D_a ($\mu\text{g}/\text{m}^2\text{s}$)	C_p ($\mu\text{g}/\text{m}^3$)	D_p ($\mu\text{g}/\text{m}^2\text{s}$)
0.00	1	459	0.0	435	0.0
0.01	1	439	4.4	360	3.6
0.02	1	421	8.4	308	6.2
0.05	1	374	18.7	215	10.8
0.00	6	55	0.0	65	0.0
0.01	6	55	0.5	63	0.6
0.02	6	54	1.1	61	1.2
0.05	6	54	2.7	56	2.8

v_d = dry deposition velocity

U = wind speed

C_a = SO_2 concentration due to area sources

C_p = SO_2 concentration due to point sources

D_a = deposition due to area sources

D_p = deposition due to point sources

The obvious feature of Table 3 is the decrease of concentration with increasing deposition velocity. This is expected as more and more material is deposited upstream. The amount of material deposited at any receptor is thus implicitly dependent on the upstream deposition, but is calculated at the receptor solely using the flux equation (3), i.e., the deposition velocity and the air concentration at that point. For example, with a speed of 1.5 m/s and a deposition velocity of .01 m/s, a flux of material due to area sources of 4.4 $\mu\text{g}/\text{m}^2\text{s}$ is calculated from an air concentration of 439 $\mu\text{g}/\text{m}^3$. Similarly a flux due to point sources of 3.6 $\mu\text{g}/\text{m}^2\text{s}$ is calculated from an air concentration of 360 $\mu\text{g}/\text{m}^3$. To get the total amount of material deposited, one integrates over the appropriate time period (i.e., if the probability distribution function represents one year*, the deposition fluxes of 4.4 $\mu\text{g}/\text{m}^2\text{s}$ and 3.6 $\mu\text{g}/\text{m}^2\text{s}$ yield total material deposited of $1.39 \times 10^2 \text{ g}/\text{m}^2$ and $1.14 \times 10^2 \text{ g}/\text{m}^2$ respectively, for a total of $2.53 \times 10^2 \text{ g}/\text{m}^2$ at that receptor.) The drastic reduction in concentration (and therefore deposition) for the higher wind speed is expected since the dispersion function is inversely proportional to wind speed.

* 1 year = $3.156 \times 10^7 \text{ s}$

SECTION 4

4.0 APPLICATIONS OF THE CDM MODEL

The CDM model was used for two purposes in this study:

- To develop parameterization schemes for point and area sources that could generically be applied to several MSA's.
- To test these generic algorithms on several MSA's with detailed modeling runs using site-specific meteorology.

The parameterization scheme is discussed below.

The detailed model was exercised on New Haven, CT and Pittsburgh, PA. Emissions data were obtained from the NAPAP emissions inventory. Meteorological data in the form of STAR stability wind roses were obtained from the National Climatic Center. Mean annual nocturnal and afternoon mixing heights were obtained from Holsworth (20).

Initial test runs for New Haven revealed that a calculation grid (receptor and area source emission cells) of greater than 1 km was essential in order to achieve reasonable computing times. It was found that a 5-km grid provided a workable compromise between spatial resolution and computing resources, and thus 5-km spacing was used for Pittsburgh.

Since the NAPAP inventory provides data for all sources with emissions greater than 1 ton SO_2 /year, an enormous number of point sources can result even for a single urban area (Pittsburgh, for example). Modeling of each source as an isolated point source would drain computer time, and it is recommended that smaller sources be grouped into a sources. Further, this methodology is inherently more suitable with 5-km receptor spacing, which would otherwise miss the contribution of small point sources. Accordingly, only sources with stack heights greater than 60m were treated as isolated point sources, and stacks with heights less than or equal to 60m were grouped (within same grid square) and spread out over the 5x5 emission grid square.

The Pasquill-Gifford dispersion coefficients (urban mode) were used for all area sources, while the McElroy-Pooler curves were used for point sources inside the grid. A pollutant half-life of 3 hours was assumed for SO_2 , and removal was incorporated by the exponential decay term in Equation (3).

Comparison between the detailed CDM modeling runs and the parametric model results are discussed below.

SECTION 5

5.0 MODEL PARAMETERIZATION

Stack height plays an important role in point source modeling and is the key to allocating sources into clusters or groups (area sources) and to defining important sources with impact over a wide area. Separate parameterization schemes have been developed for point and area sources, based on parametric test-case runs with the CDM model. In both cases, a basic principle is that of eliminating the use of site-specific wind roses, in favor of more regional meteorological considerations.

5.1 POINT SOURCES

The annual average point source parameterization is based on the following concepts:

- Stack height (h_g) controls the maximum annual average concentration (X_{max}/Q).
- The downwind distance at which this concentration occurs, r_{max} , is the surface distance scale length; r_{max} will depend on h_g , and concentrations downwind of r_{max} will be a function of r_{max} only. Between the stack location and r_{max} , concentrations will be approximately proportional to r_{max} .
- Differential terrain elevations are unimportant.

Such a parameterization scheme combines all stack heights into one generalized representation, and implicitly averages all wind directions. For an urban area with many point sources of varying heights and locations, it is anticipated that errors incurred from one source will be cancelled by the others, so that no net bias will be introduced. Figure 2 depicts the results of combining stack heights in this fashion. As shown, the total spread among various stack heights reaches a factor of about 2 at a concentration ratio of 0.01, at which point absolute levels will be quite small and the error unimportant. By averaging the concentrations at a given radius downwind for all directions, a real isopleth pattern was averaged into essentially a circular one.

This point source parameterization scheme is applicable to any set of dispersion coefficients. The current implementation uses McElroy-Pooler σ 's in keeping with current EPA regulatory policy for urban areas. Plume rise calculations are implicitly included according to Briggs (16). The following schedule of plume rise parameters was used as a function of stack height in developing the parameterization, from CDM, following Lipfert's finding (3) that stack height is related to (boiler capacity)^{1/3}.

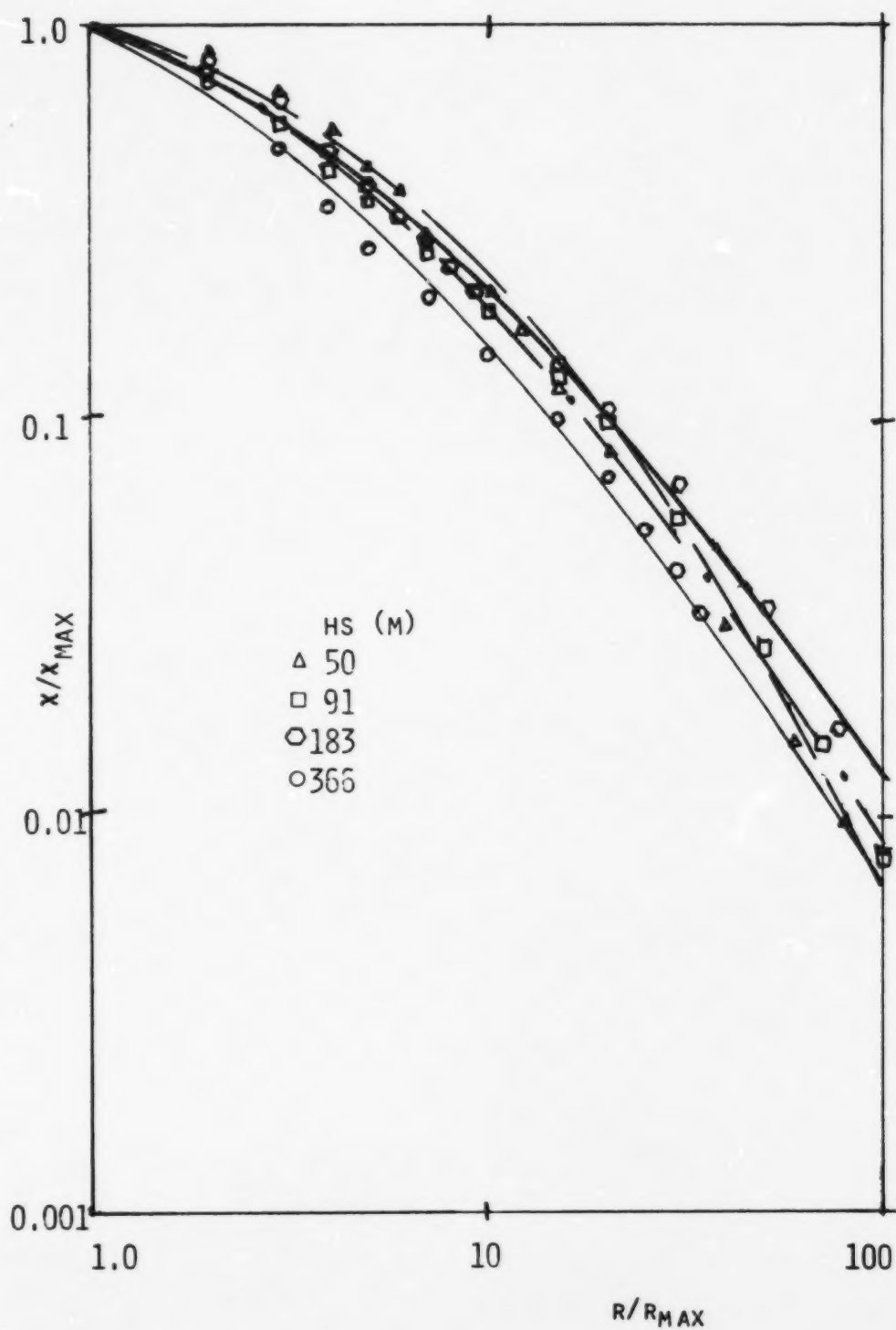


Figure 2. Concentration Ratio vs. Distance Ratio
CVG Wind Rose - Varying H_S
McElroy-Pooler σ 's.

Stack Height (m)	Stack Diameter (m)	Exhaust Velocity (m/sec)	Flue Gas Temperature (°C)
50	1.7	19.0	150
91	3.5	16.0	125
183	8.8	16.0	125
275	11.5	16.0	125
366	11.5	16.0	125

Wind rose effects are shown in Figures 3, 4, and 5. The JFK wind rose has higher wind speeds and fewer stable hours, hence the higher maximum concentrations (Figure 3). On the other hand, the downwind decay is faster. The grouping of the two interior wind rose results suggests a regionalization scheme, which has been adopted for the 1985 Assessment.

For the Northeastern U.S., two regions are defined: coastal (including Great Lakes sites) and interior or continental. The latter are characterized generally by lower wind speeds and a higher fraction of stable hours. A wind rose from JFK Airport (New York City) was used to represent Northeastern coastal sites; wind roses from Pittsburgh and Cincinnati were combined for the interior locations. PAQMAN requires a selection of the appropriate parameterizations, according to MSA location. Future assessments covering larger regions may require additional meteorological regions to be defined. Graphical representations of the applicable wind roses are presented in the Appendix.

5.2 AREA SOURCES

Area sources present a somewhat more difficult problem to generalize. First, consideration was limited to squares, in keeping with the gridding concept. Non-directional isopleth averaging was employed, as with the point source parameterization. A large number of cases was studied using CDM and arbitrary, regular configurations of varying emissions density, in order to develop some parameterization hypotheses. These were:

- Emissions density and scale length (grid size) are the primary controlling parameters for peak and grid-square-average concentrations (Figure 6).
- Concentration patterns tend to "flow" from areas of high emission density into adjacent areas of lower density, but not vice versa. This was deduced from parametric calculation runs on CDM using concentric square "rings" of varying emissions density, with higher emissions densities either on the inside or outside.

The effect of scale length on area source concentrations is an important and fundamental concept. The concentration at a particular receptor due to area source emissions, as computed in CDM, involves the computation of an average area source emission rate (q_k) at various increments of distance upwind of the receptor. This is accomplished by angular integration (narrow plume

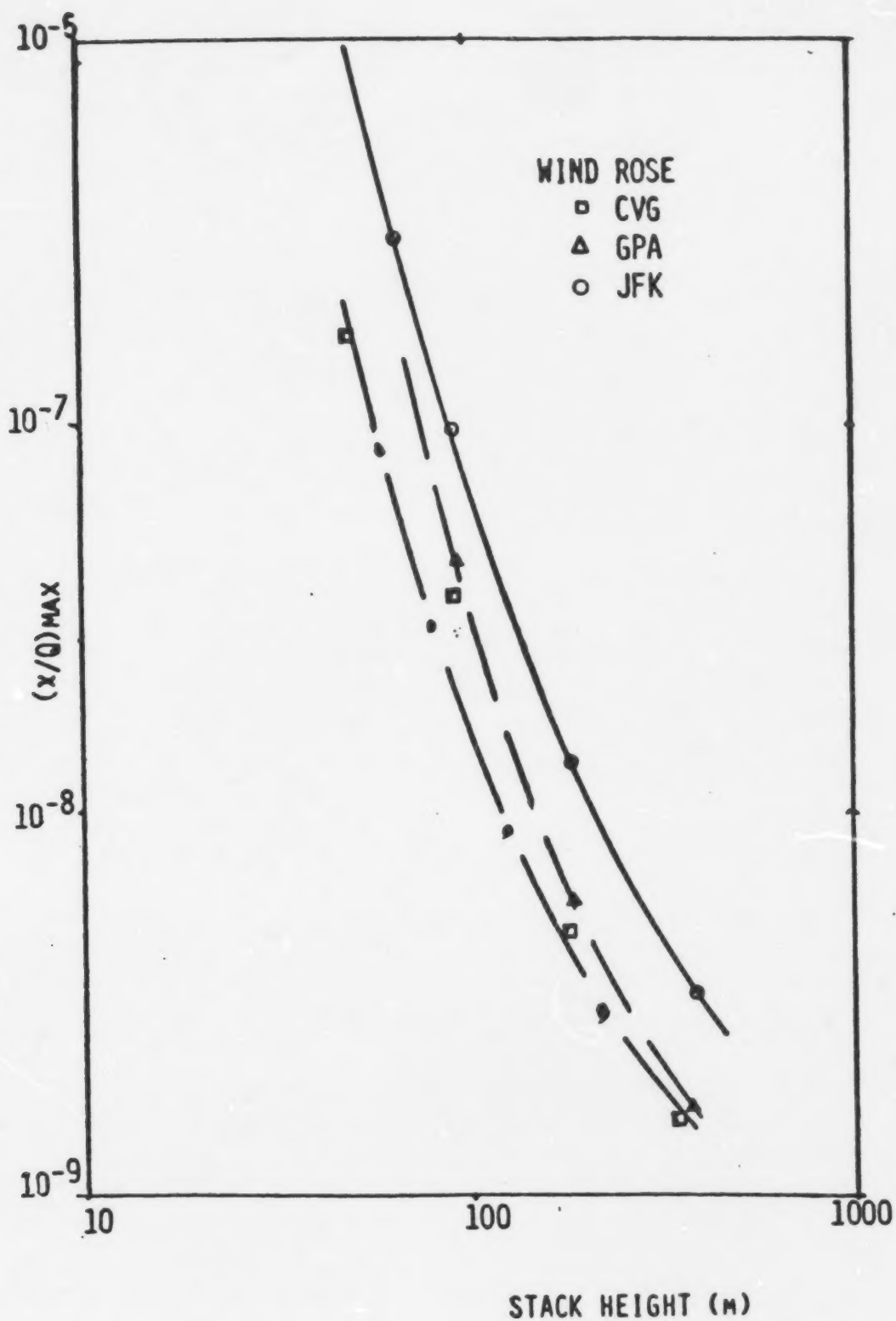


Figure 3. Maximum Concentration vs. Stack Height
 CDM Model
 McElroy-Pooler σ 's

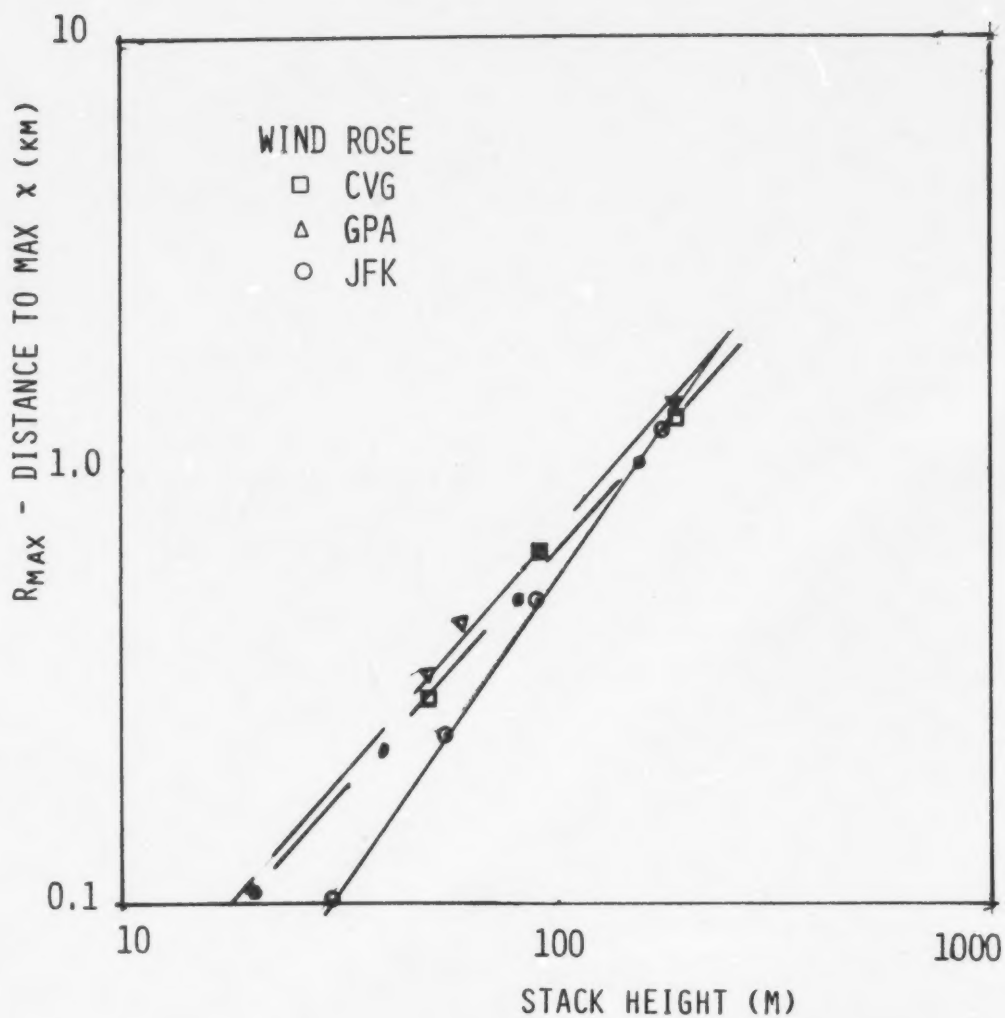


Figure 4. Downwind Distance to Maximum Concentration
CDM Model
McElroy-Pooler σ 's

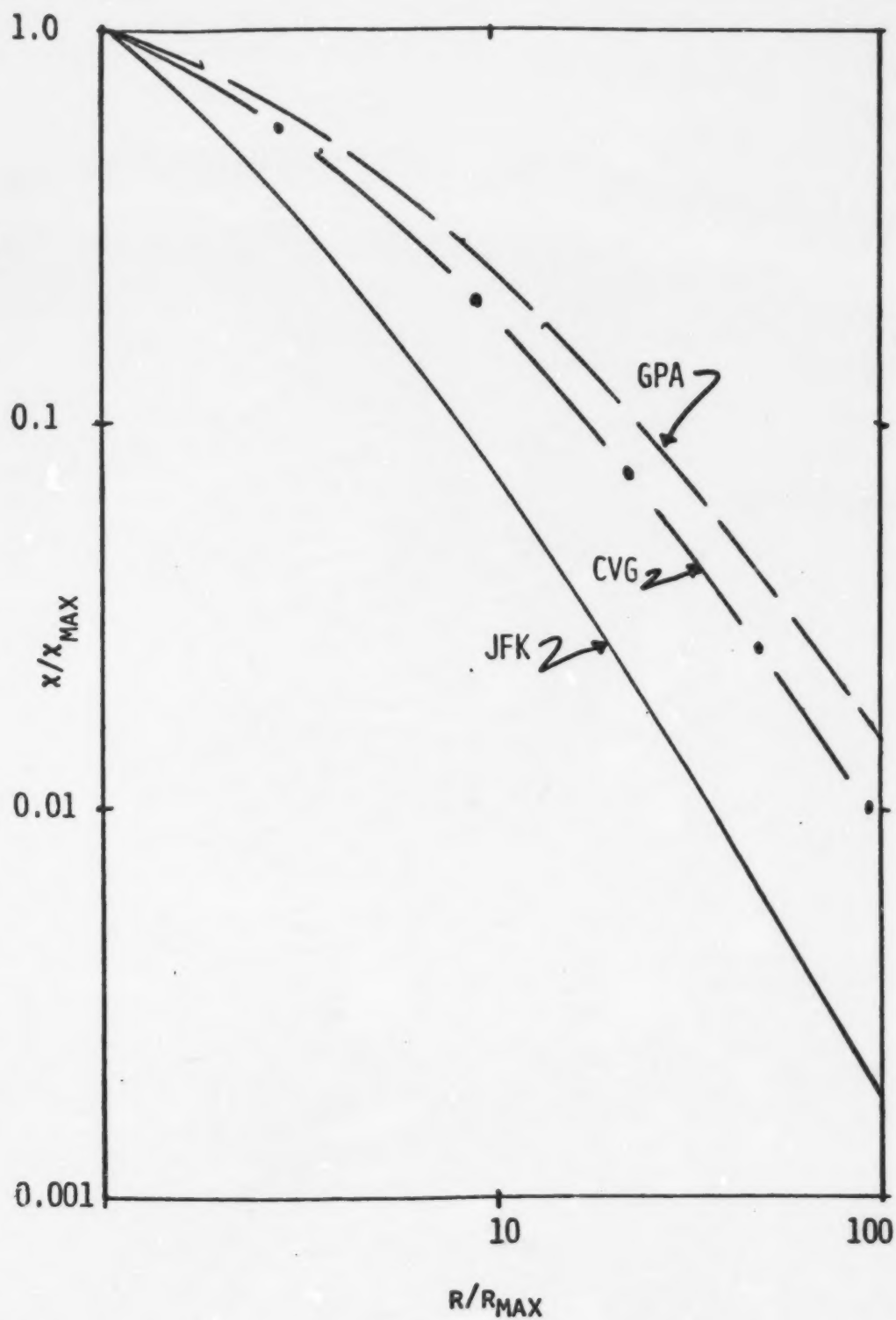


Figure 5. Concentration Ratio vs. Distance Ratio
 CDM Model
 McElroy-Pooler σ 's

hypothesis) using a sample of values of area source emission rates (input into the model by the user) along the sector arc at each distance. The degree of detail used in specifying these emission rates (i.e., the spatial extent to which these emissions are representative) will affect the concentration values computed from area sources, as shown in Figure 6. As the size of an area source shrinks (scale length decreases) at constant emission density, it approximates a point source of effectively zero strength. On the other hand, with increasing scale length (greater area), larger absolute amounts of emissions are involved and the variability of wind speed and direction during the year insures that the impact of the source will be felt somewhere within its boundaries more often. The effect dampens with larger length scales (>20 km, for example) apparently because of the non-linearities in the P-G dispersion curves.

The effect of scale length and recommendations for scale length to be used in CDM have been discussed by Irwin and Brown (21). They caution that increasing the emissions grid size (scale length) increases the similarity between adjacent grid square emissions, and much of the detail of the emission patterns within the urban center is thereby lost. (It is primarily for this reason that a simple box model was not used in our approach.) Fine spatial detail (scale length of 1-5 km) is recommended. As discussed above, parametric CDM area source runs revealed that 5-km emission grids offered a reasonable compromise between spatial detail and computing resources. Thus, the value of $\overline{XA/Q}$ (s/m) with a scale length of 5 km from Figure 6 is multiplied by the emission density (Q/A) of each area source grid in the parametric model.

Results from other urban modeling exercises in the literature are also plotted in Figure 6. Holzworth (20) used his own urban area source model, treating the city as a continuous series of infinitely long line sources, and emphasized the role of mixing height. His results were remarkably invariant over much of the Eastern U.S. on the basis of median $\overline{X/Q}$, which values have been approximated on Figure 6 for the two scale lengths he chose. Evidently meteorological variability is relatively unimportant in this region, which finding led to the concept of parameterization of a simple area source model. The results shown for Lipfert et al. (6) were computed hour-by-hour, using a relatively crude integration scheme for a circular area source and Pasquill-Gifford σ 's.

The interaction of adjacent computational grid squares is being approximated in the following way, using the concept of neighboring grid squares, as shown in Figure 7. Each grid square or cell has eight neighbors, the emissions from which are averaged to form an average "neighboring" emissions density (ED). If the central cell's ED exceeds its neighbors' (a tolerance of 10% is used), it is assumed that the local ED is operative for that cell and that the neighbors have no influence. If the neighbors' ED is the same as the interior cell (within $\pm 10\%$), the entire 9 square assemblage is treated as one unit at three times the scale length (Figure 6). If the center cell has a lower ED than its neighbors', a new weighted average ED is computed for the center cell, including the neighbors, but Figure 6 is entered using only the single cell scale length (5 km). This rather empirical calculation

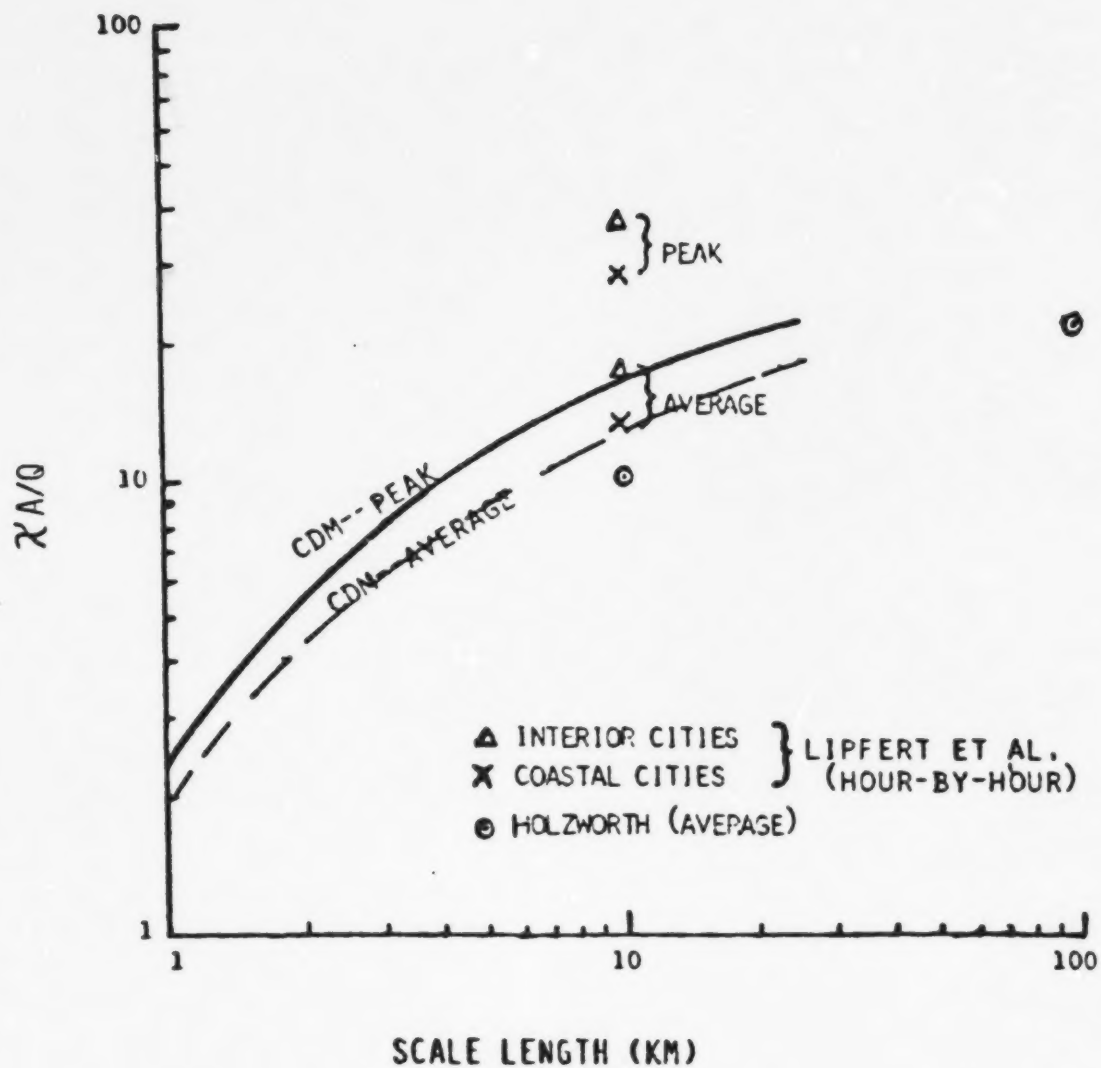
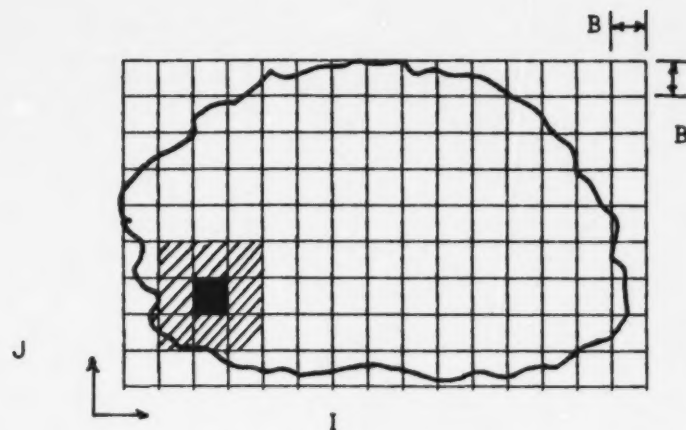


Figure 6. Scale Effect on Area-Source Diffusion
(Various Models and Wind Roses)



- FOR ISOLATED CELL, $\frac{X A}{Q} = F(B)$ (SCALE LENGTH)
 - DEFINE $\left(\frac{Q}{A}\right) N_{IJ}$ = AVERAGE OF 8 NEIGHBORING CELLS
(OFF GRID, $Q=0$)
 - TEST $(Q/A)_{IJ} - \left(\frac{Q}{A}\right) N_{IJ} = D$
- IF $D \geq 0.1$, $X_{IJ} = \left(\frac{Q}{A}\right)_{IJ} \cdot F(B)$
- IF $-0.1 \geq D \geq 0.1$, $X_{IJ} = \left\{ \frac{\left(\frac{Q}{A}\right)_{IJ} + 8 \left(\frac{Q}{A}\right) N_{IJ}}{9} \right\} \cdot F(3B)$
- IF $D < 0.1$, $X_{IJ} = \left\{ \frac{\left(\frac{Q}{A}\right)_{IJ} + 8 \left(\frac{Q}{A}\right) N_{IJ}}{9} \right\} \cdot F(B)$

Figure 7. Area Source Algorithm

algorithm was developed from parametric area source calculations and tested against actual CDM runs for New Haven and Pittsburgh, as discussed in Section 6.

5.3 SOURCE ALLOCATION ALGORITHM

It is intended that these simple concentration estimation algorithms be driven by individual stack emissions data, from the NAPAP Emissions Inventory. We are currently using Version 2.0, since it has had missing stack height data filled with estimates by SIC code, by Terry Clark of EPA. There are over 250,000 individual source records in this file, and it is important to select the minimum number that are actually applicable to each MSA in question. The procedure adopted is given below.

Each MSA consists of a listing of census tracts which are identified by centroid coordinates, among other data. A rectangular box is defined that encompasses this assemblage of points in two-dimensional space (flat earth), as shown in Figure 7. Some portions of the actual tracts may lie outside this grid, but each tract centroid is labelled with its land area and state location. This box is divided into a grid of $m \times n$ cells, about 5 km each side. They are identified with a matrix notation (i,j) and census tracts are assigned to each cell according to centroid location, together with their spatial and demographic properties.

The emission source file is sorted in similar fashion. An outer rectangle is defined by adding 50 km to each side of the MSA grid. Sources within this outer envelope are retained if their concentration exceeds $0.1 \mu\text{g}/\text{m}^3$ at the outer boundary of the MSA grid.

Within the MSA grid, a further breakdown of sources is performed. Sources with stacks less than or equal to 200 feet¹ (60m) high are designated area sources, and their emissions are summed and divided by the grid square area to form the emissions density variable needed for the area source algorithm (Figure 7). Sources with stack heights greater than 200 feet (60m) are further sorted as to their maximum possible SO_2 contributions. If X_{max} is less than $0.1 \mu\text{g}/\text{m}^3$, the source is dropped from further consideration for that MSA.

In order to deal with the situation where a given plant or facility may have a number of small emission sources, each of small consequence but possibly important in total, an aggregation procedure is used for all emission points within a 0.1-km radius. The emissions from these sources are summed and a weighted average stack height is defined:

$$h_{s_t} = \frac{\sum \frac{E}{h_s^2}}{\sum E}^{-\frac{1}{2}} \quad (8)$$

¹This is near the lower limit for which the McElroy-Pooler σ 's are valid in CDM.

This procedure may tend to overestimate the combined concentration if the stack heights within the groups are greatly different, but at least it will prevent groups of small sources being overlooked because each is too small.

Area source SO₂ emissions due to space heating are also estimated for each grid square, based on census statistics for types of fuel used. It is assumed that only fuel oil and kerosene¹ contribute SO₂ emissions, and that these contributions may be apportioned according to the spatial distribution of housing units. An average sulfur content of heating oil of 0.2% is assumed for all residential housing units; this approach assumes that any savings in heating efficiency in multiple housing units is cancelled by the use of dirtier fuels (in large apartment buildings, for example). The model has the capability to incorporate geographic trends in annual heating degree days and in average residential heated floor space, both of which are proportional to annual fuel use and thus space heating SO₂ emissions. It should be noted that space heating SO₂ emissions are a very minor component of the emissions inventory except in very densely populated areas.

The contribution of commercial and industrial buildings not captured by the point source inventory is also neglected using this approach. However, on a city-wide basis, less than 10% of all buildings are in these categories, so that this error is probably within the error bounds of the assumptions as to sulfur content and fuel use rates.

5.4 EMISSIONS INVENTORY QUALITY ASSURANCE

As a check on potential problems with the emissions inventory, each grid square calculated to exceed the primary ambient standard (80 µg/m³) is identified and the corresponding sources are listed. This should allow spot checks to locate stack heights that are coded too low or emissions that are too high. It will not, of course, identify gross underestimates of ambient concentrations (erroneous low emissions or high stacks). Some results of QA checking of the source file for specific locations are described in Section 6 under the respective case studies.

¹The sulfur content of natural gas is negligible in most urban areas. This approach to area source emissions neglects transportation sources, but the sulfur content of gasoline is negligible and that of diesel fuel quite small (<0.17).

SECTION 6

6.0 APPLICATIONS OF THE PARAMETRIC MODEL AND COMPARISON TO CDM RUNS

The parameterized calculational algorithms have been assembled and coded to allow estimates of gridded SO_2 concentrations to be made after specifying the MSA number to be considered. This model has been given the acronym "PAQMAN", for Parameterized Air Quality Model ANual. The basic model development was performed for New Haven, CT. Further runs and refinements were made for Pittsburgh.

6.1 NEW HAVEN CASE STUDY

Figure 8 presents a schematic of the New Haven, CT MSA and nearby major point sources. SO_2 monitoring data results are also shown. The detailed land use patterns for estimating the distribution of materials in place are shown in Figure 9; this gives an idea of the potential spatial resolution of the materials inventory, which is available on a census tract basis.

Since New Haven was the first test case site, several experimental modeling runs were performed using CDM, primarily to examine the sensitivity of predicted concentrations to spatial detail (area source emission grid sizes). In the first test run, area source emission cells varied from 1 km^2 in the urban center, where emission densities (census tract level) were quite variable, to as much as 64 km^2 in the outlying areas, where emission densities were smaller and more uniform. Calculations were performed on a 50 by 33 receptor grid with 1-km grid spacing. The results are shown in Figure 10.

Further tests revealed that a less-refined (i.e., $> 1 \text{ km}$ spacing) calculation grid (receptor and area source emission cells) was necessary in order to achieve reasonable computing times. A 5-km spaced grid provided a reasonable compromise between spatial resolution and computing resources, as shown below:

Grid Spacing	Maximum Concentrations from CDM		VAX 11-730 Computing Times
50 x 33 receptor grid 1-km grid cells	Local max	$43 \mu\text{g}/\text{m}^3$	~5 days
	Averaged over 5-km grid	$35 \mu\text{g}/\text{m}^3$	
11 x 7 receptor grid 5-km grid cells	Local max	$30 \mu\text{g}/\text{m}^3$	~30 minutes

The SO_2 distribution for New Haven computed with PAQMAN is shown in Figure 11, to depict the spatial resolution. Background SO_2 for this presentation was $16.8 \mu\text{g}/\text{m}^3$. The peak computed SO_2 value was $32 \mu\text{g}/\text{m}^3$ which compares well with CDM and with the measured value of $37 \mu\text{g}/\text{m}^3$.

In reviewing the emissions inventories for the major sources near New Haven, errors were found for the Port Jefferson power plant. Emissions from a 175-MW steam boiler (450-ft. stack) were assigned to a gas turbine (36-ft. stack) and vice versa. These errors were corrected for the data shown in Figure 11.

NEW HAVEN — WEST HAVEN, CT

Power Plants

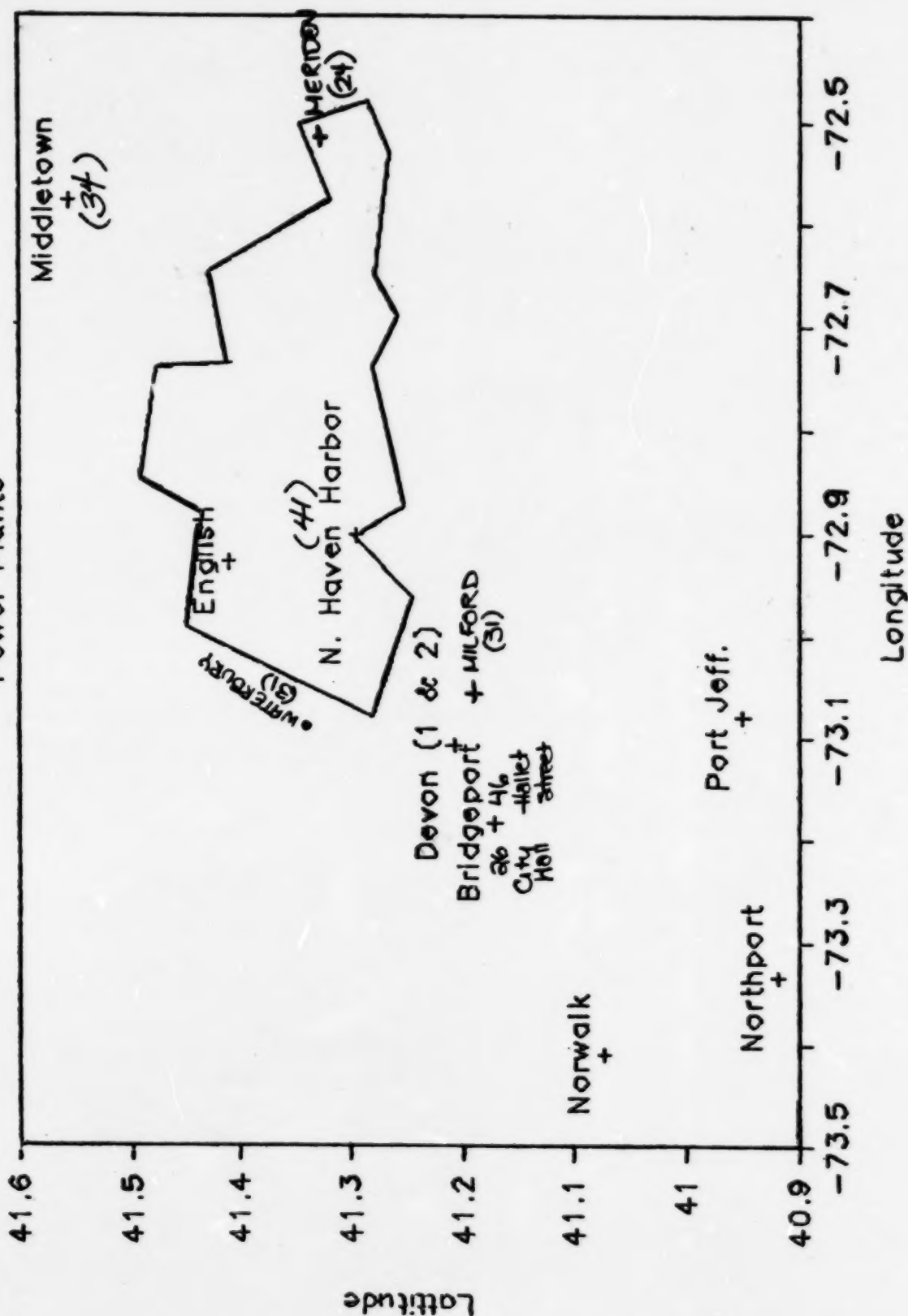
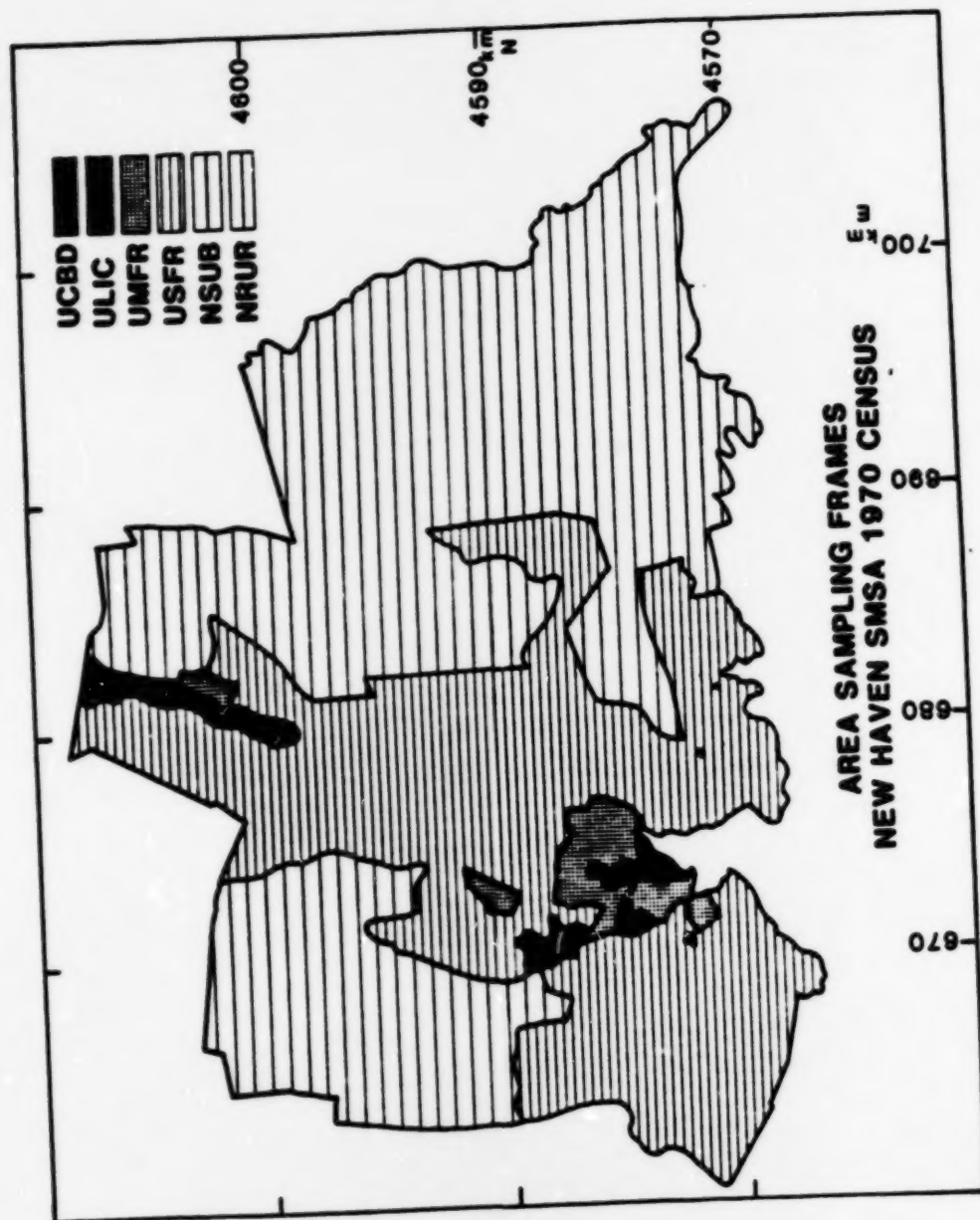


Figure 8. Schematic of the New Haven Area



Area sampling frames determined from clustering of full tracts for the New Haven SMSA, based on the 1970 census data.

Figure 9. Land Use Categories

MAXIMUM = $26 \mu\text{g}/\text{m}^3$

MAXIMUM WITH BACKGROUND ($17 \mu\text{g}/\text{m}^3$) = $43 \mu\text{g}/\text{m}^3$

MEASURED = $37 \mu\text{g}/\text{m}^3$

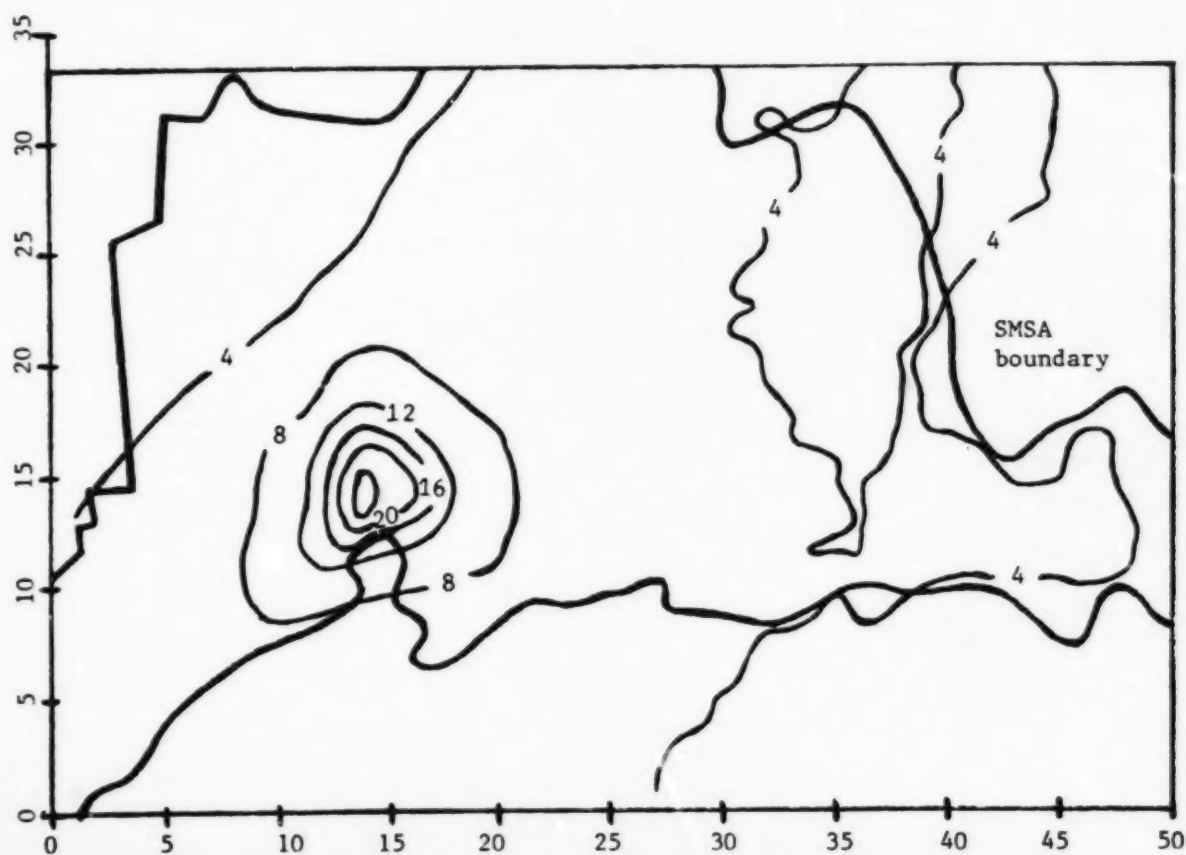


Figure 10. CDM Computed SO_2 Concentrations in New Haven, CT ($\mu\text{g}/\text{m}^3$)

NEW HAVEN — WEST HAVEN, CT

Total SO₂ — micrograms/cubic meter

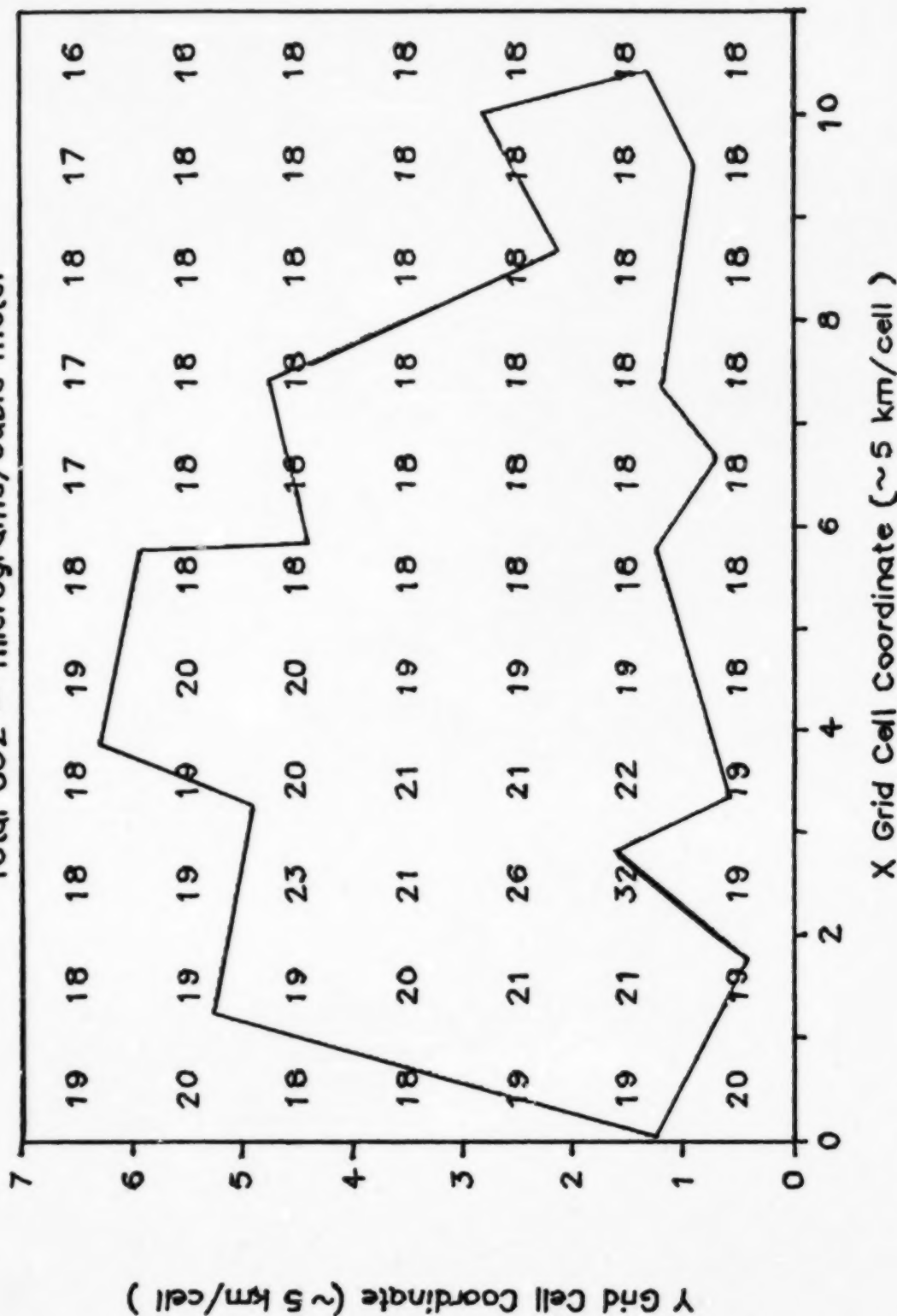


Figure 11. Total SO₂ New Haven, CT - PAQMAN

Comparison between concentrations predicted by CDM using a 5-km grid and SO₂ values predicted by PAQMAN are shown in Figure 12. The scatter plot shows good agreement, (correlation coefficient is 0.90, mean square error is 0.9 $\mu\text{g}/\text{m}^3$), particularly for the highest concentrations. The under-estimation of PAQMAN with respect to CDM at the lower concentration levels reflects the effect of our decision to ignore wind direction effects in favor of averaging in the PAQMAN algorithms. The values at the lower levels generally represent point source effects. Since New Haven is affected by point sources primarily to the west-southwest, PAQMAN tends to underpredict SO₂ contributions from these sources, as prevailing winds are from the west-southwest. The directional effect is accounted for in the CDM model.

6.2 PITTSBURGH CASE STUDY

Several test-case runs with CDM and PAQMAN were performed for the Pittsburgh MSA. The PAQMAN algorithm was utilized using both the interior and coastal algorithms. The CDM runs consisted of treating the point sources outside of the MSA grid with the P-G dispersion coefficients and the McElroy-Pooler dispersion coefficients. McElroy-Pooler was used for all point sources inside the MSA grids.¹ This presents a matrix of PAQMAN vs. CDM comparisons, as summarized in Table 4.

The results were somewhat variable, but the PAQMAN interior wind rose option produced the better one-to-one correspondence (slope >0.90) with CDM. The scatter plot for the PAQMAN interior vs. CDM (all McElroy-Pooler) is shown in Figure 13. This plot represents the other matrix combinations as well in that the largest discrepancies between the models occurred at the lower end of the scale (lower concentrations) while the models agreed very well at the hot spots. It is interesting to note that the largest differences occurred at the edge of the SMSA grid, and this may indicate that sources outside of the grid may have to be treated differently, particularly if they are located in more rural areas.

Although the root mean squared error for PAQMAN prediction vs. CDM prediction is somewhat larger than we would like (7 $\mu\text{g}/\text{m}^3$), when considered in the context of the total SO₂ concentration field in Pittsburgh, the error is acceptable. The average concentration, including background, is about 55 $\mu\text{g}/\text{m}^3$. Thus 2 σ confidence limits are about $\pm 25\%$ ². The measured values vary from 38 to 122 $\mu\text{g}/\text{m}^3$ with an average of 81 $\mu\text{g}/\text{m}^3$, which indicates the importance of spatial distributions (as in New Haven) in performing assessments.

Figure 14 compares SO₂ monitoring data with both CDM and PAQMAN calculations, both on the basis of grid square averages. There were two grid squares in the Pittsburgh area with more than one monitor (one with 2, one with 4). The

¹It should be noted that a serious error was found in the NAPAP emissions for the Pittsburgh SMSA. A reported stack height of 66m should have been 366m. This change was incorporated for both the PAQMAN and CDM runs.

²These are the limits of precision. This will correspond to accuracy as well, if PAQMAN is calibrated to CDM using the slope and intercept shown in Table 4.

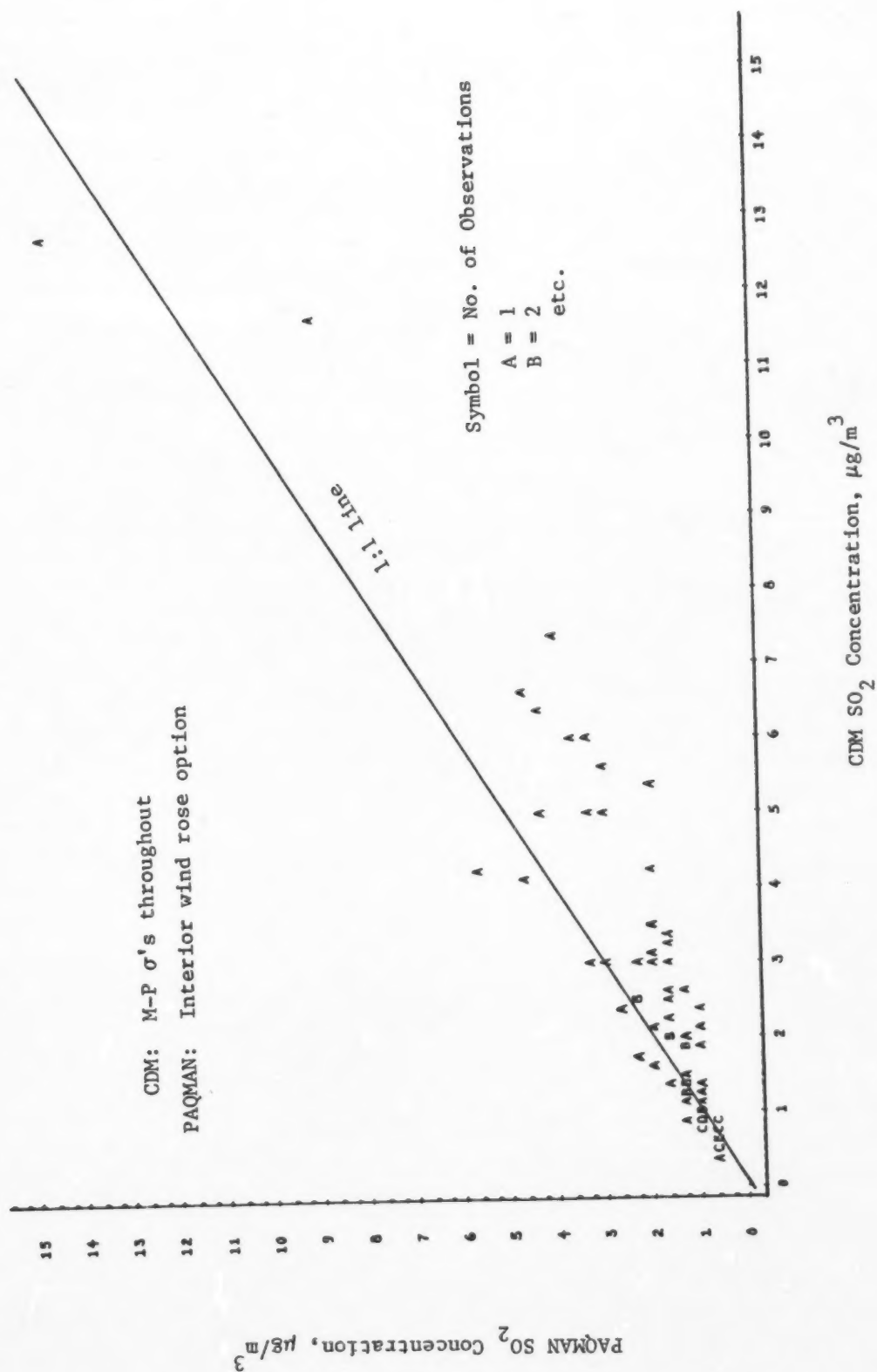


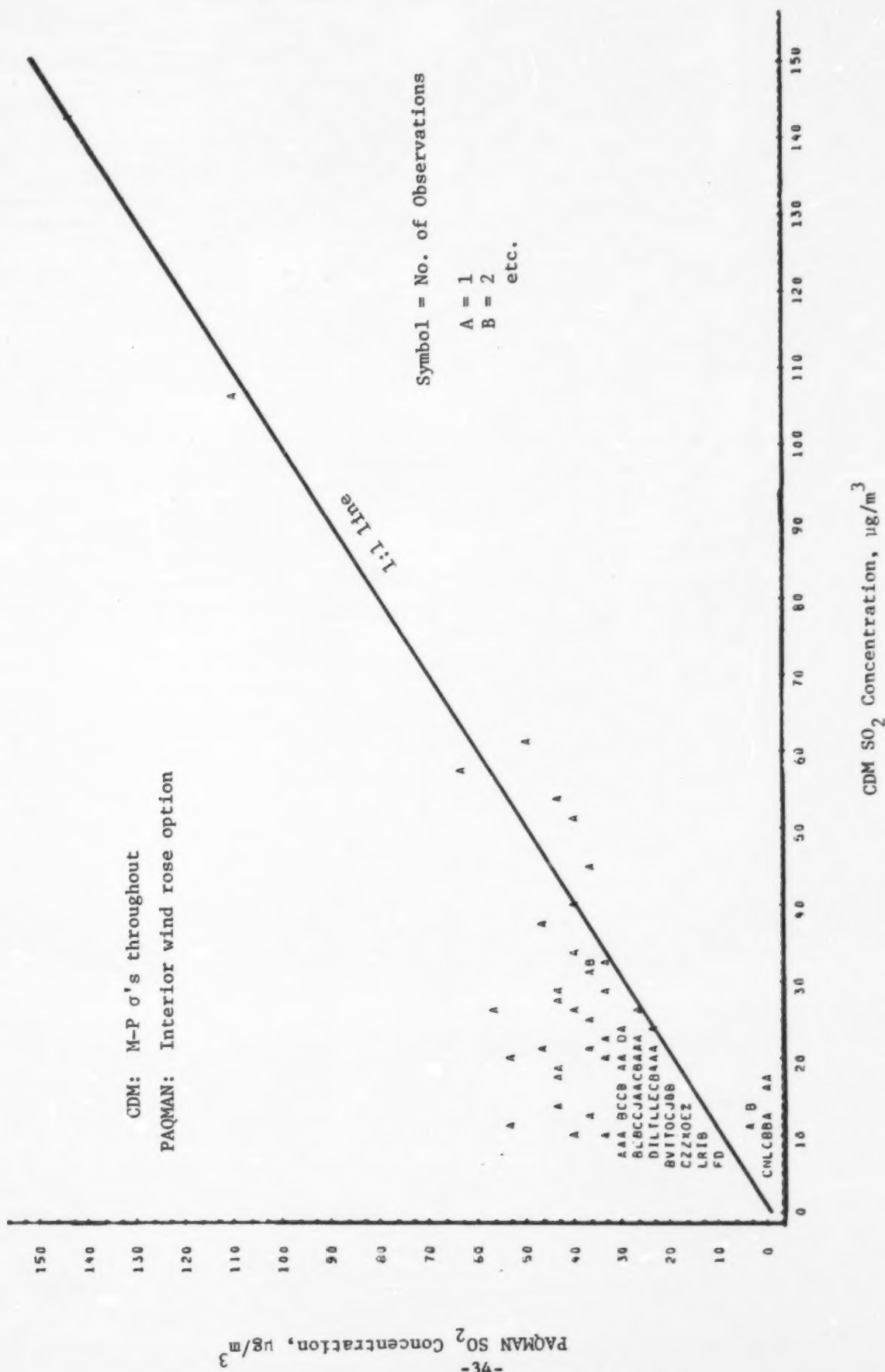
Figure 12. Comparison of PAQMAN and CDM SO₂ Concentration Estimates for New Haven

TABLE 4. REGRESSION ANALYSIS PAQMAN VS. CDM CONCENTRATIONS

PAQMAN = Dependent Variable

Operational Mode		Regression Results				Average over Grid	
PAQMAN	CDM	SLOPE m	INTER- CEPT b	CORRELA- TION COEF- FICIENT R	RMSE μg/m ³	PAQMAN (μg/m ³)	CDM (μg/m ³)
Interior Mode	M-Pσ _s Inner Grid Pt. Srcs.						
	M-Pσ _s Outer Grid Pt. Srcs.	.927	8.93	.800	6.925	20.08	12.02
Coastal Mode	M-Pσ _s Inner Grid Pt. Srcs.						
	M-Pσ _s Outer Grid Pt. Srcs.	.817	1.70	.804	5.965	11.52	12.02
Interior Mode	M-Pσ _s Outer Grid Pt. Srcs.						
	P-Gσ _s Outer Grid Pt. Srcs.	.907	8.21	.802	6.855	20.08	13.09
Coastal Mode	M-Pσ _s Outer Grid Pt. Srcs.						
	P-Gσ _s Outer Grid Pt. Srcs.	.788	1.20	.799	6.043	11.52	13.09

$$\text{PAQMAN SO}_2 = m (\text{CDM SO}_2) + b$$



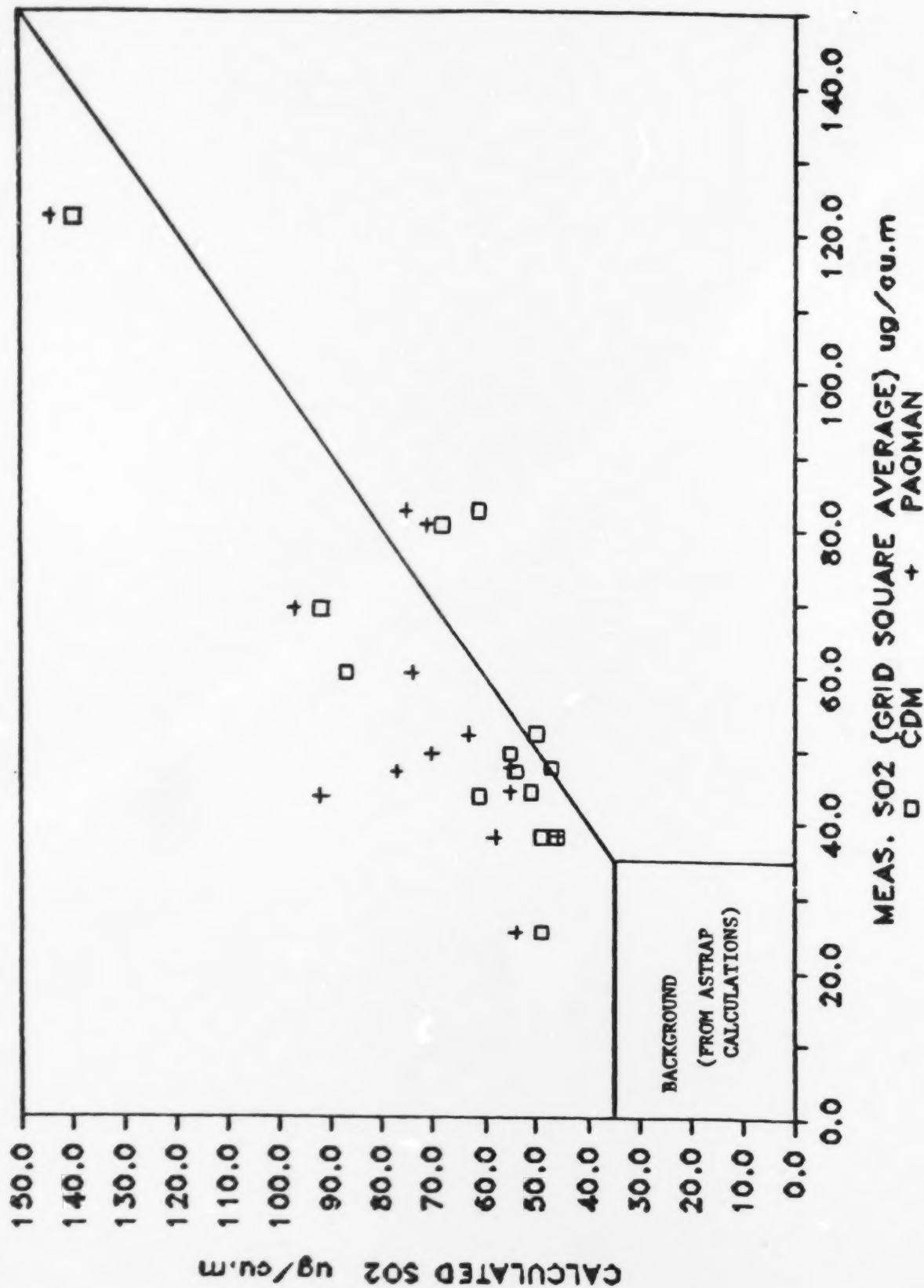


Figure 14. Calculated vs. Measured SO₂ for Pittsburgh

variation within grid squares was large when high values were encountered, reflecting the impact of local sources. However, overall, the comparison is reasonable both with respect to the background estimate (only one measured value below this level) and the high concentrations (note excellent agreement between the two models). Comparisons to monitoring data are difficult in an area like Pittsburgh where air quality has been improving markedly in recent years; the emissions inventory contains stack emissions data as old as 1970, and thus probably represents an overestimate of ca. 1980 emissions and hence air quality. Some SO₂ monitoring stations in Pittsburgh show a drop by a factor of 2 from 1977 to 1982.

All things considered, PAQMAN does a good job of predicting the high SO₂ concentrations, but tends to be more sensitive to the model's averaging of wind directional effects (point sources) at the lower levels. In terms of an overall assessment, the error is not serious, but we intend to continue to seek improvements in the parameterization scheme.

SECTION 7

7.0 LIMITATIONS OF THE MODEL

While the parameterization model (PAQMAN) performed well for the two case studies analyzed here, there are limitations to its application in certain circumstances. Many of the limitations are characteristic of the CDM model from which PAQMAN is derived. The following should be noted:

- The model is only geared for flat terrain cases, and its applicability to urban areas of complex terrain (mountainous or hilly) is unknown. CDM is strictly a flat-terrain model; thus a new guideline model should be mimicked for locations where terrain is important.
- Since the model is structured to be "meteorology-free", its applicability to locations frequently subject to specialized meteorological conditions such as wind channeling (up or down a valley) or fumigation is also questionable. Situations where channeling effects result in a site-specific prevailing wind pattern and increased wind speeds in a given direction may require a more detailed analysis than can be provided using the algorithms derived in this study. Similarly, the parameterization model does not account for effects due to fumigation since the relationships between stack height, ground-level concentration and source-receptor distances are different under these conditions. Although in many cases fumigation effects may be smoothed out over a long-term annual average, certain locations (along a shoreline) are more prone to such episodes at certain times of the year. The effect of such conditions, however, would decrease with increasing distance from the shoreline, and inland sources (>5 km) are not likely to be affected, especially on a long-term basis. Sources in mountainous valleys are also subject to fumigation when surface nocturnal inversions, formed by cool air drainage into the valley, begin to erode from heating of the surface.
- Since the parameterization scheme combines all stack heights into one generalized representation, it is expected (and apparent from the comparison results) that errors incurred from one source will be effectively cancelled by the others, eliminating any net bias, when applied to an urban area with many point sources of varying heights and locations. This may not be the case if the model is applied to isolated point sources.
- The sensitivity of our decision to classify all sources with stack heights ≤ 200 feet as area sources, regardless of emission rate, needs to be examined. The area source algorithms used in the CDM model are gross simplifications of the complex dispersion characteristic of low-level emission releases, and appreciable differences in concentrations have been shown depending on whether a source is treated as an area or point source in the model.

It should be noted that for most of the urban areas in the U.S., these limitations are not very serious, especially for the Northeast where terrain features are moderate. However, for future applications to the West, some consideration should be given to appropriate improvements in the parameterizations.

SECTION 8

8.0 REGIONAL BACKGROUND AIR QUALITY AND WET DEPOSITION

This project requires regional background air quality and wet deposition of H^+ in order to drive the materials damage functions. The following methods have been adopted to meet those needs.

8.1 BACKGROUND SO_2

The procedure outlined above results in concentration estimates only for the "local" and "nearby" sources of SO_2 .¹ In many cases, regional background is an important portion of the total observed concentration. Estimates of these background concentrations were provided by Dr. Jack Shannon of Argonne National Laboratory, using the ASTRAP model and 1980 North American emissions. Figure 15 presents a plot of these background SO_2 data, consisting of annual averages derived from seasonal calculations.

Local source contributions were excluded from the ASTRAP calculations by use of a grid system, about 115 km on a side. For each grid square, only the emissions sources outside that square were included in the calculation. Since calculations were made at ASTRAP grid cell centroids, the non-local or regional sources were 55-80 km away or more (a range is used since the cells vary in size and were rectangular, not circular). These background data compare quite well with the monitoring data, as seen for example in Figure 14 for Pittsburgh.

8.2 HYDROGEN ION (H^+) DEPOSITION ESTIMATES

H^+ deposition data were obtained from the Acid Deposition Systems (ADS) based on monitoring data for 1982. The data were interpolated to a 1/2 degree latitude-longitude grid based on a kriging procedure (22). Isopleths are shown in Figure 16. This grid was then interpolated for each MSA in the 17 states considered in this assessment. No adjustments for urban influences were made, following a recommendation by Dr. Ari Patrinos of BNL.

The rationale for this decision is as follows. The average measured SMSA SO_2 levels in the quadrant exceed background by about 80% or less, or about 20 $\mu g/m^3$. According to Lipfert et al. (23), this would correspond to an increase in precipitation sulfate of about 12 $\mu eq/l$. To estimate the average change in acidity would require estimates of urban perturbations in NO_3^- , NH_4^+ , and Ca^{++} . According to this same reference, a change in Ca^{++} of 12 $\mu eq/l$, would correspond to an urban increment in TSP of about 12 $\mu g/m^3$, a reasonable average figure for many urban areas, circa 1980. Thus the first order delta H^+ estimate for most urban areas is approximately zero.

¹"Local" is defined as sources within the rectangular envelope enclosing the MSA. "Nearby" sources are within 50 km of this boundary. All other sources are included in "regional background."



Figure 15. Background SO_2 Data ($\mu\text{g}/\text{m}^3$)
Source: ASTRAP Model Runs for 1980.

KRIGED H^+

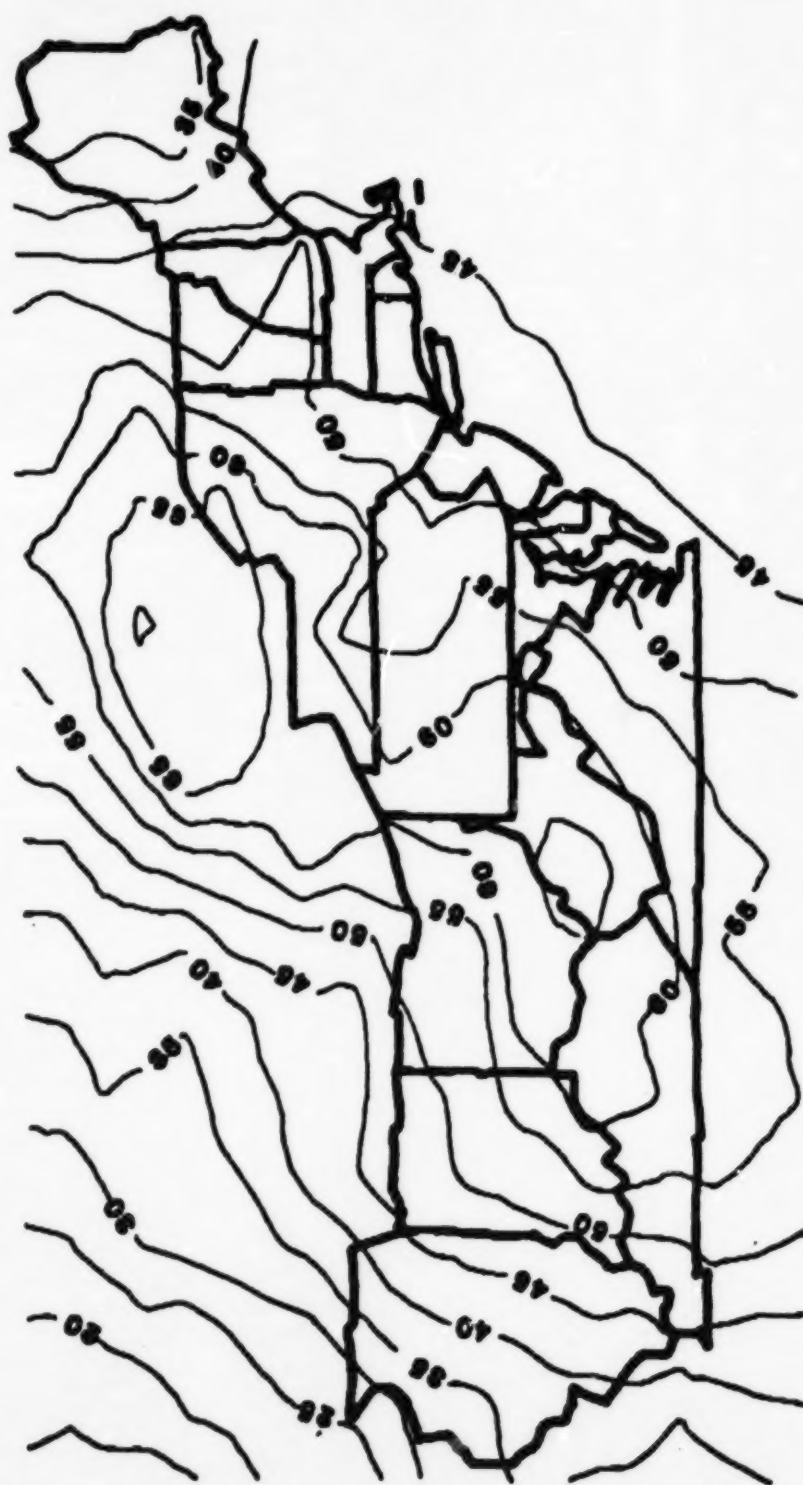


Figure 16. Hydrogen Ion Deposition Isopleths. ($mg/m^2/yr$)

SECTION 9

9.0 CONCLUSIONS

A methodology has been developed for use in materials damage assessment, providing estimates of wet and dry deposition for both urban and background areas. At this point, the estimates are limited to SO₂ air concentrations and wet deposition of hydrogen ion (H⁺).

The local air quality model for urban areas is a parameterization of the CDM model, and provides a reasonable representation of its performance at a fraction of the run time, with automated input drivers. Regional meteorology is assumed, with separate parameterization schemes for point and area sources. Accuracy estimates are about $\pm 25\%$, although the model tends to perform better at high concentrations than it does at lower levels.

REFERENCES

1. U.S. Environmental Protection Agency. Guideline on air quality models. Draft (revised). Office of Air and Radiation, Office of Air Quality Planning and Standards, USEPA, Research Triangle Park, NC, 1984.
2. Londergan, R.J., Reynolds, S.D., Seigneur, C., Stoeckenius, T.E., Moore, Gary E., and Johnson, Robert G. Operational validation of Gaussian plume models at a plains site. SYSAPP-83/172, Systems Applications, Inc., San Rafael, CA, 1983.
3. Lipfert, F.W. Regional issue identification and assessment program (RIIA) Issue Paper 5: A methodology for analyzing the short-term air quality impacts of new power plants. BNL 51292, Brookhaven National Laboratory, Upton, NY, 1979.
4. Simpson, R.W., Jakeman, A.J., and Daly, N.J. The relationship between the ATDL model and the statistical distributions of wind, speed, and pollution data. Atmos. Envir. 19, No. 1, 75-82, 1985.
5. Benarie, Michel M. Urban air pollution modelling. The MIT Press, Cambridge, MA, 1980.
6. Lipfert, Frederick W., Moskowitz, Paul D., Dungan, Jennifer, Tichler, Joyce, and Carney, Thomas. The interaction between air pollution dispersion and residential heating demands. APCA J. 33, No. 3, 1983.
7. Guttman, H. Effects of atmospheric factors on the corrosion rate of rolled zinc. ASTM STP 435, 223-240, 1968.
8. Sehmel, George A. Particle and gas dry deposition: a review. Atmos. Envir. 14, 983-1011, 1980.
9. Evans, L.S., Raynor, G.S., and Jones, D.M.A. Frequency distributions for durations and volumes of rainfalls in the eastern United States in relation to acidic precipitation. Water, Air, and Soil Pollut. 23 (2), 187, 1984.
10. Wyzga, Ronald E. and Lipfert, Frederick W. Forecasting materials damage from air pollution. Paper for presentation at 78th Annual Meeting of the Air Pollution Control Association, Detroit, Michigan. June 16-21, 1985.
11. Lipfert, F.W., Benarie, M., and Daum, M.L. Derivation of metallic corrosion damage functions for use in environmental assessments. Draft Report, in preparation. Brookhaven National Laboratory, Upton, NY.
12. Dopazo, C., Lee, H-N, and Michael, P. Brookhaven National Laboratory long-term Gaussian dispersion model. BNL-24226, Brookhaven National Laboratory, Upton, NY, 1977.
13. TRW Systems Group. Air quality display model. PB-189194. Prepared for Dept. of Health, Education and Welfare, U.S. Dept. of Commerce, Springfield, VA, 1969.

14. U.S. Environmental Protection Agency. User's guide for the climatological dispersion model. Environmental Monitoring Series. EPA-R4-73-024. Research Triangle Park, NC, 1973.
15. Bowers, J.F., Bjorklund, J.R., and Cheney, C.S. Industrial source complex (ISC) dispersion model user's guide, Vol. I. EPA-450/4-79-030, (NTIS PB80-133044). Source Receptor Analysis Branch, U.S. Environmental Protection Agency, Research Triangle Park, NC, 1979.
16. Briggs, G.A. Plume Rise. AEC Critical Review Series. TID-25075, 1969.
17. Briggs, G.A. Plume rise predictions, lectures on air pollution and environmental impact analysis. D.A. Haugen, ed. American Met. Soc., Boston, MA, 59-111, 1975.
18. Holland, J.Z. A meteorological survey of the Oak Ridge area. Atomic Energy Commission, Report ORO-99, 554-559, 1953. 584 pp.
19. Turner, D.B., Zimmerman, J.R., and Busse, A.D. An evaluation of some climatological dispersion models. Third Meeting of the NATO/CCMS Panel on Modeling, Paris, France, 1972.
20. Holzworth, G.C. Mixing heights, wind speeds, and potential for urban air pollution throughout the contiguous United States. Environmental Protection Agency, January 1972.
21. Irwin, J.S. and Brown, T.M. A sensitivity analysis of the treatment of area sources by the climatological dispersion model, JAPCA, 35:359-364, 1985. U.S. Environmental Protection Agency, Research Triangle Park, NC.
22. Olsen, A.R., and Watson, C.R. Data quality screening criteria and summary measures. Memorandum, Battelle Pacific Northwest Laboratories, 1984.
23. Lipfert, F.W., Dupuis, L.R., and Alvarez, L. Urban and local source effects on precipitation chemistry. BNL 34565. Presented at 77th Air Pollution Control Assoc. Annual Meeting, San Francisco, CA, June 24-29, Preprint No. 84-21.3, 1984, 19 pp.

APPENDIX A

WIND ROSE COMPARISONS

Directional wind roses for Pittsburgh (GPA), Cincinnati (CVG) and New York (JFK) are presented graphically in the form of histograms in Figures A-1 through A-3. The wind roses are sorted by atmospheric stability and wind speed since these parameters are essentially the driving forces of the CDM model, and are summarized for all wind directions in Table A-1.

The results depict a clear distinction between JFK (coastal) and the two inland sites. JFK is characterized by far fewer stable hours (only 30%) than Pittsburgh (57%) or Cincinnati (56%), and about two times the occurrence of neutral hours (58% versus 29% and 27% at Pittsburgh and Cincinnati, respectively). This is likely the effect of increased wind speeds due to local sea breezes and to a lesser extent coastal storms (since they occur less frequently than the sea breeze). Indeed, this is apparent from the wind speed distributions, which show a greater occurrence of strong and moderate winds at JFK, and fewer occurrences of higher winds related to the two inland sites.

The strong similarities between Pittsburgh and Cincinnati support a regional meteorological approach, at least for cities inland and west of the Appalachians. These similarities also explain the similar relationships between stack height and ground-level concentration that were found using each of the wind roses in the CDM model.

The differences between CVG/GPA and JFK imply that separate algorithms are needed for coastal areas. Distributions from additional locations need to be analyzed to determine if additional meteorological regions need to be defined.

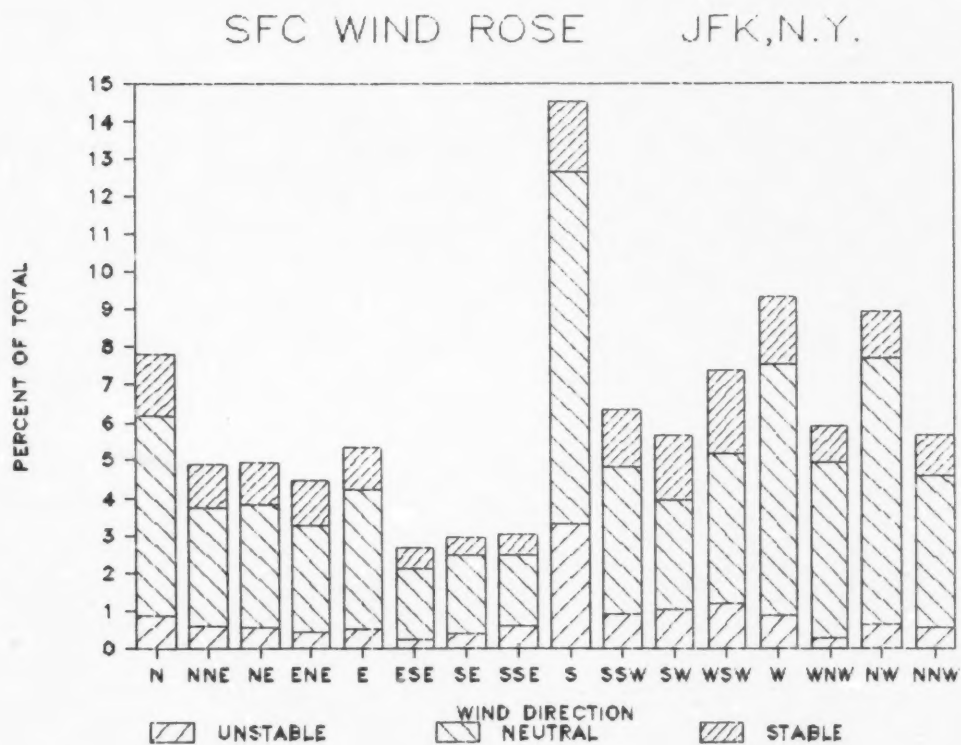
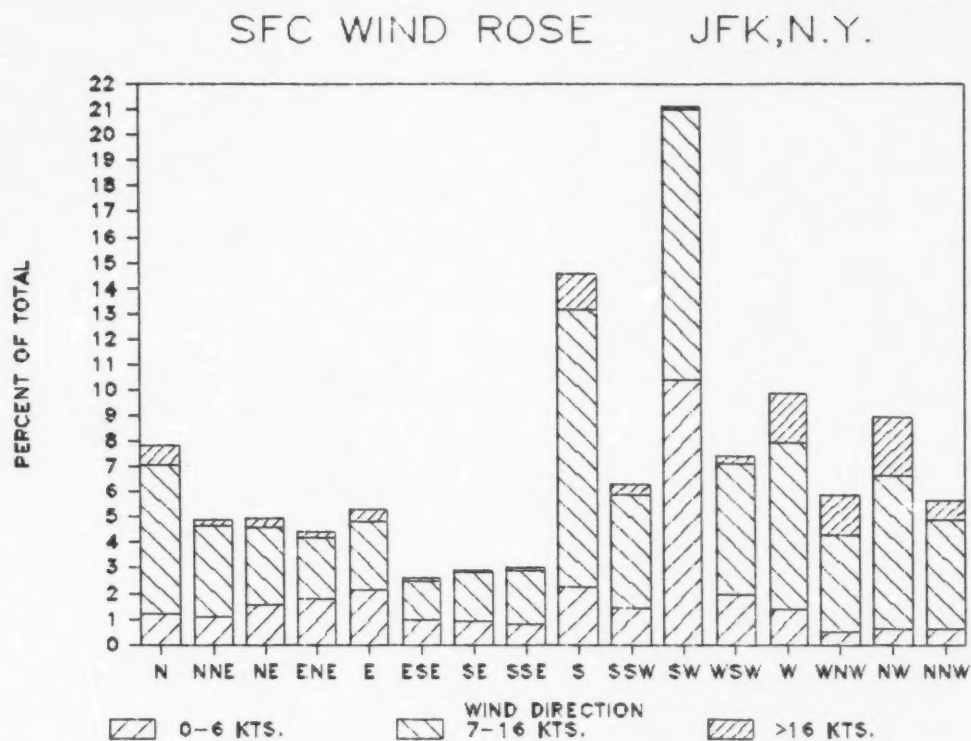
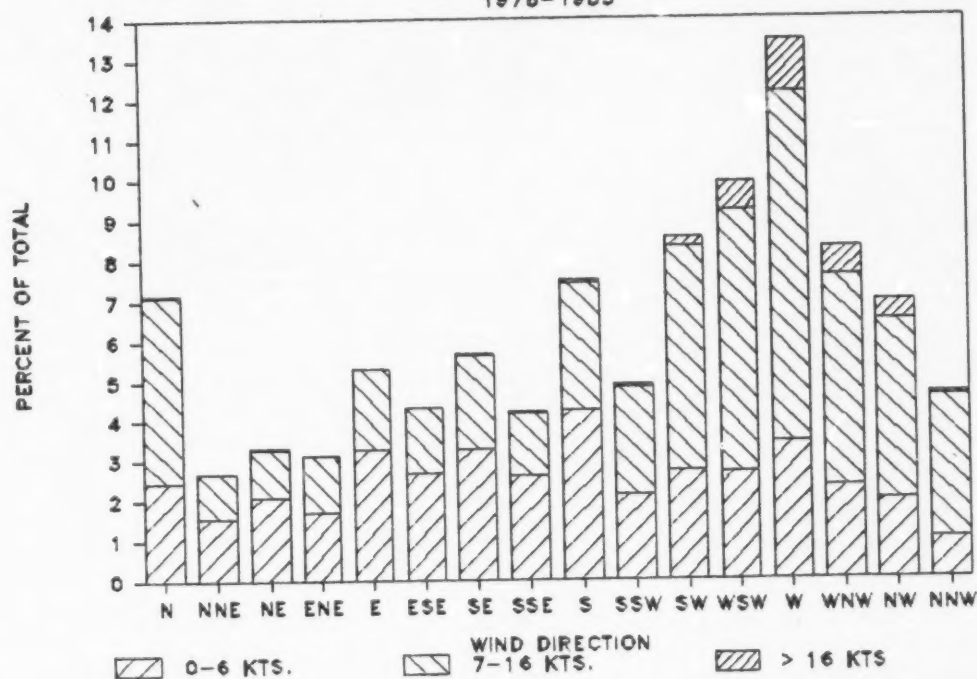


Figure A-1. Surface Wind Roses by Stability and Wind Speed.

SFC WIND ROSE PITTSBURGH, PA. 1978-1983



SFC WIND ROSE PITTSBURGH, PA. 1978-1983

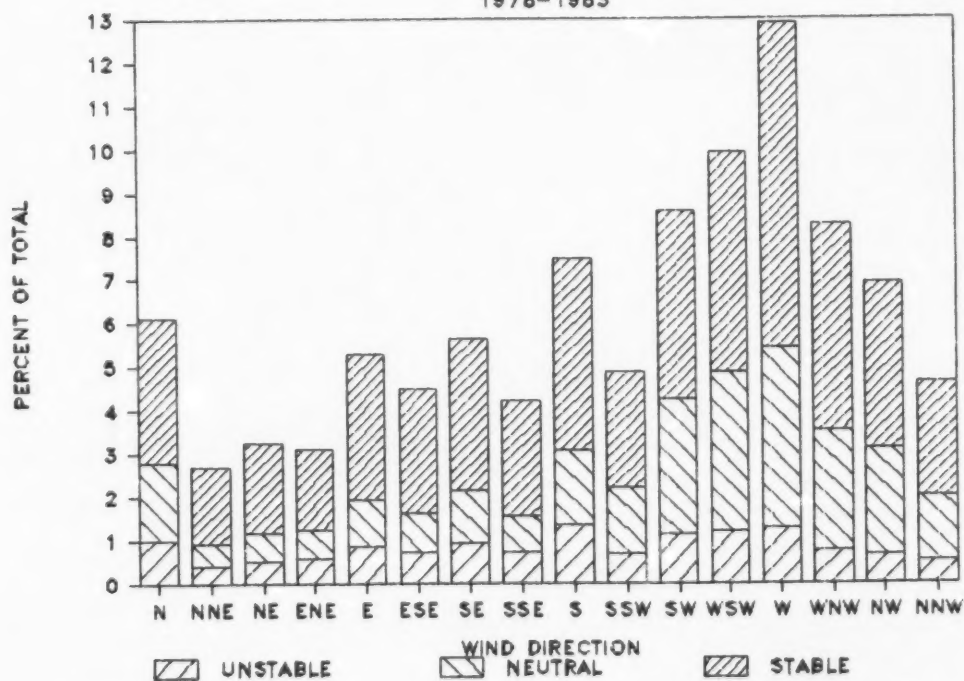


Figure A-2. Surface Wind Roses by Stability and Wind Speed

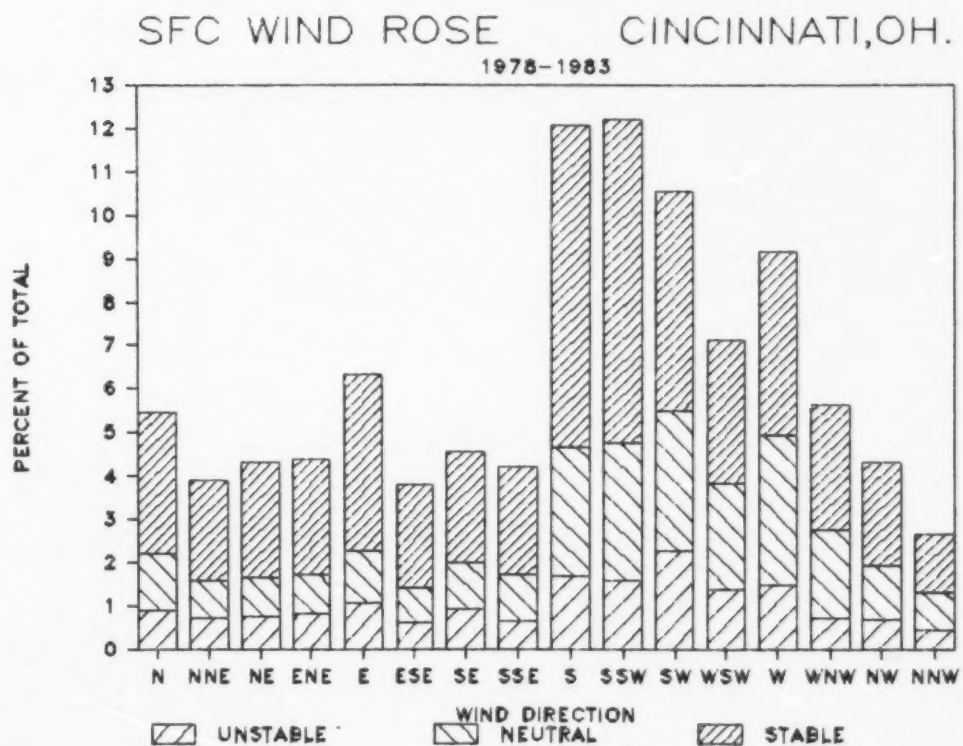
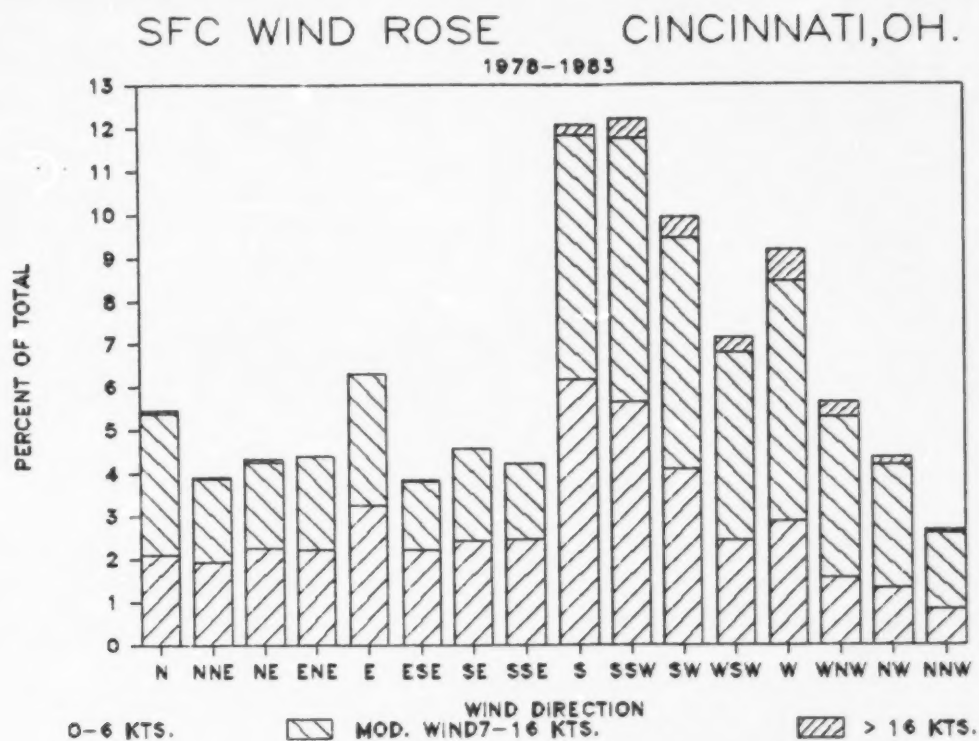


Figure A-3. Surface Wind Roses by Stability and Wind Speed.

TABLE A-1 WIND ROSE STATISTICS

<u>Percent Occurrence - Stability</u>			
	<u>Unstable</u>	<u>Neutral</u>	<u>Stable</u>
New York (JFK)	12	58	30
Pittsburgh (GPA)	14	29	57
Cincinnati (CVG)	17	27	56

<u>Wind Frequency Distribution Summary</u>			
<u>Site</u>	<u>Percent Occurrence - Wind Speed (Kts)</u>		
	<u>0-6</u>	<u>7-10</u>	<u>>16</u>
New York (JFK)	25	65	10
Pittsburgh (GPA)	40	56	4
Cincinnati (CVG)	49	53	3

APPENDIX B

PAQMAN USER'S GUIDE

Brookhaven National Laboratory's Parameterized Air Quality Model, Annual (PAQMAN) is written in non-standard FORTRAN 77 for a Digital Equipment Corporation VAX series computer. Modifications to the software will be necessary to operate the model on other computer systems. The user should consult his/her FORTRAN 77 programmer's guide and computer operation manual to modify and/or execute the program.

Model Description

The various components of the PAQMAN model have been discussed in the main text. A flow chart of the source allocation algorithms is shown in Figure B-1. A complete listing of the program is provided in Appendix C.

Model Input Requirements

The model is specifically designed to operate with a minimum of user input requirements. A flag, indicating which set of dispersion algorithms (those based on coastal meteorology or interior meteorology) is desired, is chosen by the user depending upon the location of the city in question. Additional inputs consist only of the MSA code, and filenames of the census tract and SO₂ receptor data sets. Format specifications are shown in Figure B-2.

In areas such as the urban Northeast, where several MSA's "neighbor" each other, the model combines the individual MSA's into one large MSA. The user simply enters the MSA codes sequentially for each MSA, followed by the end of MSA indicator, as shown in Figure B-3.

Variable Description	Format	Example
Meteorology Flag*	—	COASTAL
MSA Code	I4	5600
End of MSA Code Indicator	I4	Must be 0000
Census Tract Filename	—	CENSUS.DAT
SO ₂ Receptor Filename	—	SO2REC.DAT

*At present, choices are limited to COASTAL or INTERIOR meteorology.
Note: All entries must begin in Column 1.

Figure B-2. PAQMAN Input Variable Description and Format Specification

```

Column 1
↓
INTERIORW
3280  }
1170  } MSA Codes
5440  }
4960  }
0000  (end of MSA indicator)

```

Figure B-3. Example of PAQMAN Input (Actual inputs in bold)

SOURCE ALLOCATION ALGORITHM

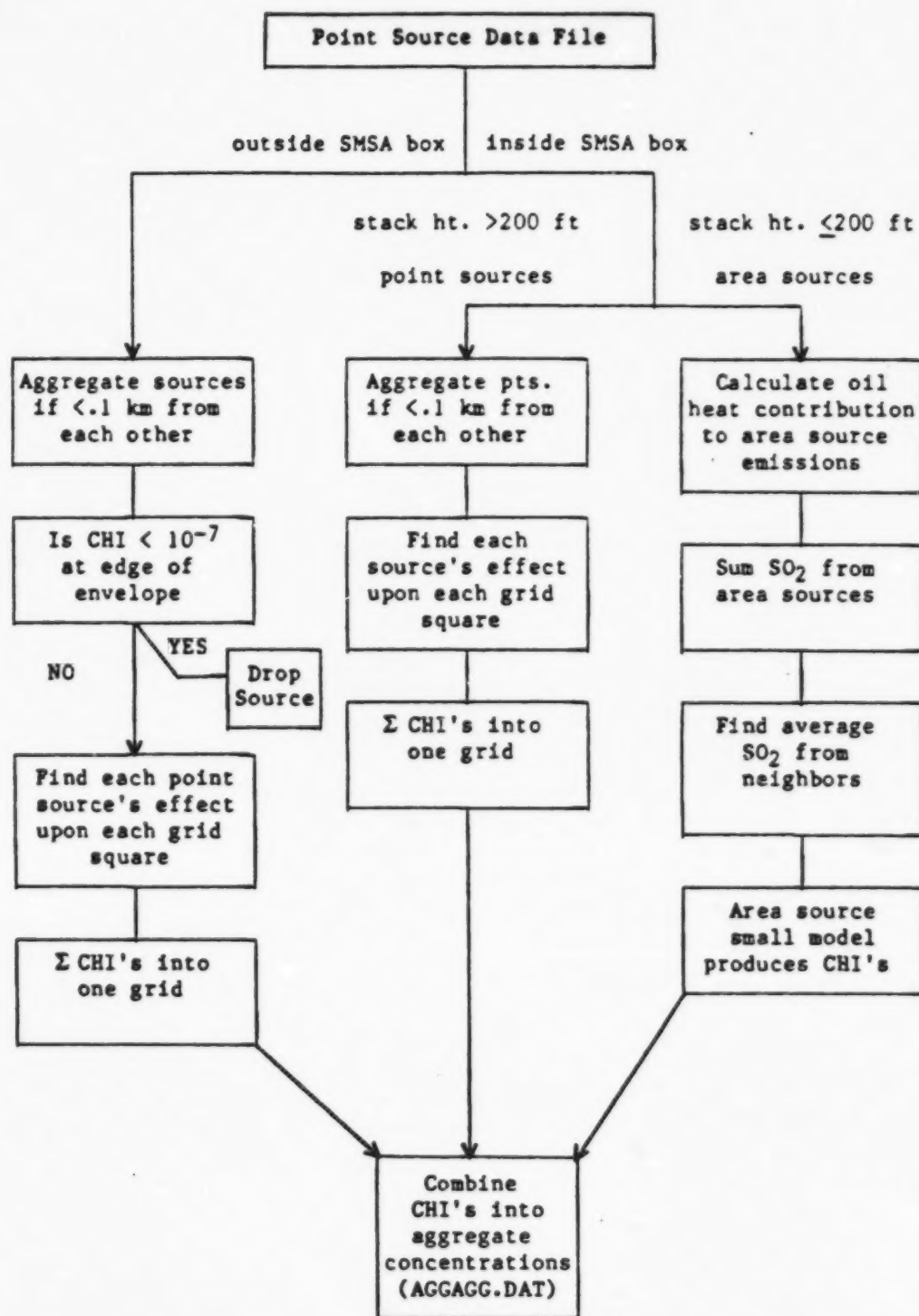


Figure B-1. PAQMAN Source Allocation Algorithm

APPENDIX C

PAQMAN PROGRAM CODE LISTING

(Available from Brookhaven National Laboratory)